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CUTINASE VARIANTS

FIELD OF THE INVENTION

The present invention relates to a cutinase variant, more particularly to a 5 cutinase variant having improved thermostability. The invention also relates to a DNA sequence encoding the variant, a vector comprising the DNA sequence, a transformed host cell harboring the DNA sequence or the vector, to a method of producing the variant, and to use of the variant.

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BACKGROUND OF THE INVENTION

Cutinases are lipolytic enzymes capable of hydrolyzing the substrate cutin. Cutinases are known from various fungi (P.E. Kolattukudy in "Lipases", Ed. B. Borgström and H.L. Brockman, Elsevier 1984, 471-504). The amino acid sequence and the crystal structure of a cutinase of Fusarium solani pisi have been described (S. Longhi et al., Journal of Molecular Biology, 268 (4), 779-799 (1997)). The amino acid 15 sequence of a cutinase from Humicola insolens has also been published (US 5,827,719).

A number of variants of the cutinase of Fusarium solani pisi have been published: WO 94/14963; WO 94/14964; Appl. Environm. Microbiol. 64, 2794-2799, 1998; Proteins: Structure, Function and Genetics 26, 442-458, 1996; J. of Computational 20 Chemistry 17, 1783-1803, 1996; Protein Engineering 6, 157-165, 1993; Proteins: Structure, Function, and Genetics 33, 253-264, 1998.

Fungal cutinases may be used in the enzymatic hydrolysis of cyclic oligomers of poly(ethylene terephthalate), e.g. in the finishing of yarn or fabric from poly(ethylene terephthalate) fibers (WO 97/27237). However, it is desirable to improve the thermo-25 stability of known fungal cutinases to allow a higher process temperature.

SUMMARY OF THE INVENTION

The inventors have found certain variants of fungal cutinases having improved thermostability.

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Accordingly, the invention provides a variant of a parent fungal cutinase comprising substitution of one or more amino acid residues which is located:

- a) within 17 Å from the location of the N-terminal amino acid (as calculated from amino acid residues in a crystal structure), and/or
- b) within 20 positions from the N-terminal amino acid.

The invention also provides a DNA sequence encoding the variant, an expression vector comprising the DNA sequence, a transformed host cell harboring the DNA sequence or the expression vector, and a method of producing the variant by cultivating the transformed host cell so as to produce the variant and recovering the variant from the resulting broth. The invention also provides a process for enzymatic hydrolysis of cyclic oligomers of poly(ethylene terephthalate) by treatment with the cutinase variant and a detergent composition comprising the variant.

BRIEF DESCRIPTION OF THE DRAWINGS

Fig. 1 shows the 3D structure of the cutinase of *H. insolens*.

Fig. 2 is a computer model showing the three-dimensional structures of the cutinases from *F. solani pisi* (left) and *H. insolens* (right). Different colors have been used to identify the N-terminal amino acid and zones of 12 Å and 17 Å diameter around this.

Figs. 3-6 illustrate the hydrolysis of c3ET. Details are given in the Examples.

20 DETAILED DESCRIPTION OF THE INVENTION

Fungal cutinase

The parent cutinase is a fungal cutinase, particularly a filamentous fungal cutinase, preferably native to a strain of *Humicola* or *Fusarium*, more preferably *H. insolens* or *F. solani pisi*, most preferably *H. insolens* strain DSM 1800.

The amino acid sequence of the cutinase of *H. insolens* strain DSM 1800 and the DNA sequence encoding it are shown as SEQ ID NO: 2 and SEQ ID NO: 1 of US 5,827,719. The numbering system used herein for the *H. insolens* cutinase is based on the mature peptide, as shown in said SEQ ID NO: 2.

The amino acid sequence of the cutinase of F. solani pisi is shown as the mature peptide in Fig. 1D of WO 94/14964. The numbering system used herein for the F. solani pisi cutinase is that used in WO 94/14964; it includes the pro-sequence shown in said Fig. 1D; thus, the mature cutinase is at positions 16-214.

The parent cutinase preferably has an amino acid sequence which is at least 50 % (particularly at least 70 % or at least 80 %) homologous to the cutinase of H. insolens strain DSM 1800. Preferably, the parent cutinase is one that can be aligned with the cutinase of H. insolens strain DSM 1800.

Homology and alignment

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For purposes of the present invention, the degree of homology may be suitably determined according to the method described in Needleman, S.B. and Wunsch, C.D., (1970), Journal of Molecular Biology, 48, 443-45, with the following settings for polypeptide sequence comparison: GAP creation penalty of 3.0 and GAP extension penalty of 0.1. The determination may be done by means of a computer program 15 known such as GAP provided in the GCG program package (Program Manual for the Wisconsin Package, Version 8, August 1994, Genetics Computer Group, 575 Science Drive, Madison, Wisconsin, USA 53711).

Two given sequences can be aligned according to the method described in Needleman (supra) using the same parameters. This may be done by means of the 20 GAP program (supra)...

Three-dimensional structure of cutinase

The structure of the cutinase of H. insolens was solved in accordance with the principle for X-ray crystallographic methods as given, for example, in X-Ray Structure Determination, Stout, G.K. and Jensen, L.H., John Wiley & Sons, Inc. NY, 1989. The 25 structural coordinates for the solved crystal structure at 2.2 Å resolution using the isomorphous replacement method are given in Fig. 1 in standard PDB format (Protein Data Bank, Brookhaven National Laboratory, Brookhaven, CT).

The structure of the cutinase of F. solani pisi is described in Martinez et al. (1992) Nature 356, 615-618. The 3D structures of the cutinases of F. solani pisi and H. insolens are compared as a computer model in Fig. 2.

It should be noted that the overall three-dimensional structure of the fungal cutinases is very similar and has been shown by X-ray crystallography to be highly homologous. The similarities between the cutinases from F. solani pisi and H. insolens is clearly apparent from the computer model in Fig. 2. It is therefore to be expected that modifications of the type indicated for one fungal cutinase will also be functional for other fungal cutinases.

Substitution near N-terminal

The variant of the invention has one or more amino acid substitutions in the vicinity of the N-terminal. The substitution is within a distance of 17 Å (preferably within 12 Å) and/or within 20 positions (preferably within 15 positions) of the N-terminal. The distance from the N-terminal is to be calculated between the Cα atom of the amino acids, and is calculated from an amino acid in a crystal structure (i.e. visible in the X-ray structure).

In the cutinase of *H. insolens* strain DSM 1800, the two N-terminal amino ac15 ids Q1 and L2 are not visible in the X-ray structure, so the distance is to be calculated from amino acid G3. Amino acids within 17 Å include positions 3-12, 18, 20-60, 62-64, 82, 85-86, 100-108, 110-111, 130-132, 174, 176-182, 184-185, 188, and 192. Those within 12 Å include positions 3-8, 22-27, 30-47, 53-59, 102, 177, and 180-181.

In the cutinase of *F. solani pisi*, the N-terminal amino acid G17 is visible in the 20 X-ray structure. Amino acids within 17 Å include positions 17-26, 34-75, 77-79, 101, 115, 117-119, 147, 191-197, 199-200, and 203. Those within 12 Å include positions 17-22, 38, 40, 45-58, 60, 65, and 70-72.

The variants of the invention have improved thermostability compared to the parent enzyme. The thermostability may be determined from the denaturation temperature by DSC (differential scanning calorimetry), e.g. as described in an example, e.g. at pH 8.5 with a scan rate of 90 K/hr. Preferred variants have a denaturation temperature which is at least 5°C higher than the parent enzyme.

The total number of substitutions in the above regions is typically not more than 10, e.g. not more than substitutions in the above regions. In addition, the cutinase variant of the invention may optionally include other modifications of the parent enzyme, typically not more than 10, e.g. not more than 5 alterations (substitutions,

deletions or insertions) outside of the above regions. Thus, the total amino acid sequence of the variant may have not more than 20, e.g. not more than 10 alterations compared to the parent cutinase.

Solvent accessible surface

One or more of the substitutions is preferably made at an exposed amino acid residue, i.e. an amino acid residue having a solvent accessible surface. This can be calculated by teh "dssp" program (version October 1988) described in W. Kabsch and C. Sander, Biopolymers, 22 (1983) pp. 2577-2637.

In the cutinase of *H. insolens* strain DSM 1800, the following amino acids lie within 17 Å of G3 at the N-terminal and have a solvent accessible surface greater than 0: 3-12, 18, 26-33, 36-38, 40-45, 47-56, 59-60, 62-64, 82, 85-86, 104-105, 174, 176-179, 181-182, 192.

Preferred substitutions

A preferred substitution near the N-terminal is one that increases the electrical charge, i.e. a substitution of a negatively charged amino acid with a neutral or positively charged amino acid or substitution of a neutral amino acid with a positively charged amino acid. This substitution may be made at a position corresponding to position E6, E10, E47 or E179 in the cutinase of *Humicola insolens* strain DSM 1800, preferably a substitution corresponding to E6Q, E10Q, E47K or E179Q.

Another preferred substitution near the N-terminal is substitution with a Pro residue, preferably a substitution corresponding to A14P or R51P in the cutinase of *Humicola insolens* strain DSM 1800.

Preferred variants

The following are some preferred variants in the *H. insolens* cutinase. Corre²⁵ sponding variants of other parent cutinases are also preferred. (JC numbers are the inventors' designations).

JC006: R51P

JC011: E6Q, L138I

JC013: A14P, E47K

JC014, JC015: E47K

JC025: E179Q

JC026: E6Q, E47K, R51P

JC029: A14P, E47K, E179Q

JC030: E47K, E179Q

JC031: E47K, D63N

JC038: E6Q, A14P, E47K, R51P, E179Q

JC039: E6Q, E10Q, A14P, E47K, R51P, E179Q

JC040: Q1P, L2V, S11C, N15T, F24Y, L46I, E47K

10 Use of cutinase variant

The cutinase variant of the invention may be used, e.g., for the enzymatic hydrolysis of cyclic oligomers of poly(ethylene terephthalate), such as cyclic tri(ethylene terephthalate), abbreviated as c3ET.

In particular, this may be used to remove such cyclic oligomers from polyester containing fabric or yarn by treating the fabric or yarn with the cutinase variant, preferably followed by rinsing the fabric or yarn with an aqueous solution having a pH in the range of from about pH 7 to about pH 11. The treatment of polyester is preferably carried out above the glass transition temperature of c3ET (about 55°C) and below the glass transition temperature of polyester (about 70°C). Thus, the treatment is preferably carried out at 55-70°C, e.g. at 60-65°C. The process may be carried out in analogy with WO 97/27237.

The cutinase variant of the invention is also useful in detergents, where it may be incorporated to improve the removal of fatty soiling, as described in WO 94/03578 and WO 94/14964.

25 Nomenclature for amino acid alterations

The nomenclature used herein for defining mutations is basically as described in WO 92/05249. Thus, R51P indicates substitution of R in position 51 with P.

Methods for preparing cutinase variants

The cutinase variant of the invention can be prepared by methods known in the art, e.g. as described in WO 94/14963 or WO 94/14964 (Unilever). The following describes methods for the cloning of cutinase-encoding DNA sequences, followed by methods for generating mutations at specific sites within the cutinase-encoding sequence.

Cloning a DNA sequence encoding a cutinase

The DNA sequence encoding a parent cutinase may be isolated from any cell or microorganism producing the cutinase in question, using various methods well known in the art. First, a genomic DNA and/or cDNA library should be constructed using chromosomal DNA or messenger RNA from the organism that produces the cutinase to be studied. Then, if the amino acid sequence of the cutinase is known, labeled oligonucleotide probes may be synthesized and used to identify cutinase-encoding clones from a genomic library prepared from the organism in question. Alternatively, a labeled oligonucleotide probe containing sequences homologous to another known cutinase gene could be used as a probe to identify cutinase-encoding clones, using hybridization and washing conditions of lower stringency.

Yet another method for identifying cutinase-encoding clones would involve inserting fragments of genomic DNA into an expression vector, such as a plasmid,
transforming cutinase-negative bacteria with the resulting genomic DNA library, and
then plating the transformed bacteria onto agar containing a substrate for cutinase
(i.e. maltose), thereby allowing clones expressing the cutinase to be identified.

Alternatively, the DNA sequence encoding the enzyme may be prepared synthetically by established standard methods, e.g. the phosphoroamidite method described S.L. Beaucage and M.H. Caruthers, (1981), Tetrahedron Letters 22, p. 1859-1869, or the method described by Matthes et al., (1984), EMBO J. 3, p. 801-805. In the phosphoroamidite method, oligonucleotides are synthesized, e.g. in an automatic DNA synthesizer, purified, annealed, ligated and cloned in appropriate vectors.

Finally, the DNA sequence may be of mixed genomic and synthetic origin, mixed synthetic and cDNA origin or mixed genomic and cDNA origin, prepared by

ligating fragments of synthetic, genomic or cDNA origin (as appropriate, fragments corresponding to various parts of the entire DNA sequence), in accordance with standard techniques. The DNA sequence may also be prepared by polymerase chain reaction (PCR) using specific primers, for instance as described in US 5 4,683,202 or R.K. Saiki et al., (1988), Science 239, 1988, pp. 487-491.

Site-directed mutagenesis

Once a cutinase-encoding DNA sequence has been isolated, and desirable sites for mutation identified, mutations may be introduced using synthetic oligonucleotides. These oligonucleotides contain nucleotide sequences flanking the desired mu-10 tation sites. In a specific method, a single-stranded gap of DNA, the cutinaseencoding sequence, is created in a vector carrying the cutinase gene. Then the synthetic nucleotide, bearing the desired mutation, is annealed to a homologous portion of the single-stranded DNA. The remaining gap is then filled in with DNA polymerase I (Klenow fragment) and the construct is ligated using T4 ligase. A specific example of 15 this method is described in Morinaga et al., (1984), Biotechnology 2, p. 646-639. US 4,760,025 discloses the introduction of oligonucleotides encoding multiple mutations by performing minor alterations of the cassette. However, an even greater variety of mutations can be introduced at any one time by the Morinaga method, because a multitude of oligonucleotides, of various lengths, can be introduced.

Another method for introducing mutations into cutinase-encoding DNA sequences is described in Nelson and Long, (1989), Analytical Biochemistry 180, p. 147-151. It involves the 3-step generation of a PCR fragment containing the desired mutation introduced by using a chemically synthesized DNA strand as one of the primers in the PCR reactions. From the PCR-generated fragment, a DNA fragment 25 carrying the mutation may be isolated by cleavage with restriction endonucleases and reinserted into an expression plasmid.

Expression of cutinase variants

According to the invention, a DNA sequence encoding the variant produced by methods described above, or by any alternative methods known in the art, can be expressed, in enzyme form, using an expression vector which typically includes control sequences encoding a promoter, operator, ribosome binding site, translation initiation signal, and, optionally, a repressor gene or various activator genes.

Expression vector

The recombinant expression vector carrying the DNA sequence encoding a cutinase variant of the invention may be any vector which may conveniently be subjected to recombinant DNA procedures, and the choice of vector will often depend on the host cell into which it is to be introduced. The vector may be one which, when introduced into a host cell, is integrated into the host cell genome and replicated together with the chromosome(s) into which it has been integrated. Examples of suitable expression vectors include pMT838.

Promoter

In the vector, the DNA sequence should be operably connected to a suitable promoter sequence. The promoter may be any DNA sequence which shows transcriptional activity in the host cell of choice and may be derived from genes encoding proteins either homologous or heterologous to the host cell.

Examples of suitable promoters for directing the transcription of the DNA sequence encoding a cutinase variant of the invention, especially in a bacterial host, are the promoter of the *lac* operon of *E.coli*, the *Streptomyces coelicolor* agarase gene dagA promoters, the promoters of the *Bacillus licheniformis* α-amylase gene (amyL), the promoters of the *Bacillus stearothermophilus* maltogenic amylase gene (amyM), the promoters of the *Bacillus amyloliquefaciens* α-amylase (amyQ), the promoters of the *Bacillus subtilis* xylA and xylB genes etc. For transcription in a fungal host, examples of useful promoters are those derived from the gene encoding *A. oryzae* TAKA amylase, the TPI (triose phosphate isomerase) promoter from *S. cerevisiae* (Alber et al. (1982), J. Mol. Appl. Genet 1, p. 419-434, *Rhizomucor miehei* aspartic proteinase, *A. niger* neutral α-amylase, *A. niger* acid stable α-amylase, *A. niger* glucoamylase, *Rhizomucor miehei* lipase, *A. oryzae* alkaline protease, *A. oryzae* triose phosphate isomerase or *A. nidulans* acetamidase.

Expression vector

The expression vector of the invention may also comprise a suitable transcription terminator and, in eukaryotes, polyadenylation sequences operably connected to the DNA sequence encoding the α -amylase variant of the invention. Termi-5 nation and polyadenylation sequences may suitably be derived from the same sources as the promoter.

The vector may further comprise a DNA sequence enabling the vector to replicate in the host cell in question. Examples of such sequences are the origins of replication of plasmids pUC19, pACYC177, pUB110, pE194, pAMB1 and pIJ702.

The vector may also comprise a selectable marker, e.g. a gene the product of which complements a defect in the host cell, such as the dal genes from B. subtilis or B. licheniformis, or one which confers antibiotic resistance such as ampicillin, kanamycin, chloramphenicol or tetracyclin resistance. Furthermore, the vector may comprise Aspergillus selection markers such as amdS, argB, niaD and sC, a marker 15 giving rise to hygromycin resistance, or the selection may be accomplished by cotransformation, e.g. as described in WO 91/17243.

The procedures used to ligate the DNA construct of the invention encoding a cutinase variant, the promoter, terminator and other elements, respectively, and to insert them into suitable vectors containing the information necessary for replication, are 20 well known to persons skilled in the art (cf., for instance, Sambrook et al., Molecular Cloning: A Laboratory Manual, 2nd Ed., Cold Spring Harbor, 1989).

Host Cells

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The cell of the invention, either comprising a DNA construct or an expression vector of the invention as defined above, is advantageously used as a host cell in the 25 recombinant production of a cutinase variant of the invention. The cell may be transformed with the DNA construct of the invention encoding the variant, conveniently by integrating the DNA construct (in one or more copies) in the host chromosome. This integration is generally considered to be an advantage as the DNA sequence is more thely to be stably maintained in the cell. Integration of the DNA constructs into the flost chromosome may be performed according to conventional methods, e.g. by homologous or heterologous recombination. Alternatively, the cell may be transformed with an expression vector as described above in connection with the different types of host cells.

The cell of the invention may be a cell of a higher organism such as a mam-5 mal or an insect, but is preferably a microbial cell, e.g. a bacterial or a fungal (including yeast) cell.

Examples of suitable bacteria are Gram positive bacteria such as Bacillus subtilis, Bacillus licheniformis, Bacillus lentus, Bacillus brevis, Bacillus stearothermophilus, Bacillus alkalophilus, Bacillus amyloliquefaciens, Bacillus coagulans, Bacillus to circulans, Bacillus lautus, Bacillus megaterium, Bacillus thuringiensis, or Streptomyces lividans or Streptomyces murinus, or gramnegative bacteria such as E.coli. The transformation of the bacteria may, for instance, be effected by protoplast transformation or by using competent cells in a manner known per se.

The yeast organism may favorably be selected from a species of Saccharo-15 myces or Schizosaccharomyces, e.g. Saccharomyces cerevisiae.

The host cell may also be a filamentous fungus e.g. a strain belonging to a species of Aspergillus, most preferably Aspergillus oryzae or Aspergillus niger, or a strain of Fusarium, such as a strain of Fusarium oxysporium, Fusarium graminearum (in the perfect state named Gribberella zeae, previously Sphaeria zeae, synonym with Gibberella roseum f. sp. cerealis), or Fusarium sulphureum (in the prefect state named Gibberella puricaris, synonym with Fusarium trichothecioides, Fusarium bactridioides, Fusarium sambucium, Fusarium roseum, and Fusarium roseum var. graminearum), Fusarium cerealis (synonym with Fusarium crokkwellnse), or Fusarium venenatum.

In a preferred embodiment of the invention the host cell is a protease deficient or protease minus strain.

This may for instance be the protease deficient strain Aspergillus oryzae JaL 125 having the alkaline protease gene named "alp" deleted. This strain is described in WO 97/35956 (Novo Nordisk).

Filamentous fungi cells may be transformed by a process involving protoplast formation and transformation of the protoplasts followed by regeneration of the cell wall a manner known per se. The use of Aspergillus as a host micro-organism is de-

scribed in EP 238 023 (Novo Nordisk A/S), the contents of which are hereby incorporated by reference.

Method of producing the cutinase variant of the invention

In yet a further aspect, the present invention relates to a method of producing a cutinase variant of the invention, which method comprises cultivating a host cell under conditions conducive to the production of the variant and recovering the variant from the cells and/or culture medium.

The medium used to cultivate the cells may be any conventional medium suitable for growing the host cell in question and obtaining expression of the cutinase variant of the invention. Suitable media are available from commercial suppliers or may be prepared according to published recipes (e.g. as described in catalogues of the American Type Culture Collection).

The cutinase variant secreted from the host cells may conveniently be recovered from the culture medium by well-known procedures, including separating the cells from the medium by centrifugation or filtration, and precipitating proteinaceous components of the medium by means of a salt such as ammonium sulphate, followed by the use of chromatographic procedures such as ion exchange chromatography, affinity chromatography, or the like.

Expression of variant in plants

The present invention also relates to a transgenic plant, plant part or plant cell which has been transformed with a DNA sequence encoding the variant of the invention so as to express and produce this enzyme in recoverable quantities. The enzyme may be recovered from the plant or plant part. Alternatively, the plant or plant part containing the recombinant enzyme may be used as such.

The transgenic plant can be dicotyledonous or monocotyledonous, for short a dicot or a monocot. Examples of monocot plants are grasses, such as meadow grass (blue grass, Poa), forage grass such as festuca, lolium, temperate grass, such as Agrostis, and cereals, e.g. wheat, oats, rye, barley, rice, sorghum and maize (corn).

Examples of dicot plants are tobacco, legumes, such as lupins, potato, sugar beet, pea, bean and soybean, and cruciferous (family Brassicaceae), such as cauliflower, oil seed rape and the closely related model organism Arabidopsis thaliana.

Examples of plant parts are stem, callus, leaves, root, fruits, seeds, and tubers. In the present context, also specific plant tissues, such as chloroplast, apoplast, mitochondria, vacuole, peroxisomes and cytoplasm are considered to be a plant part. Furthermore, any plant cell, whatever the tissue origin, is considered to be a plant part.

Also included within the scope of the invention are the progeny of such plants, plant parts and plant cells.

The transgenic plant or plant cell expressing the variant of the invention may be constructed in accordance with methods known in the art. In short the plant or plant cell is constructed by incorporating one or more expression constructs encoding the enzyme of the invention into the plant host genome and propagating the resulting modified plant or plant cell into a transgenic plant or plant cell.

Conveniently, the expression construct is a DNA construct which comprises a gene encoding the enzyme of the invention in operable association with appropriate regulatory sequences required for expression of the gene in the plant or plant part of choice. Furthermore, the expression construct may comprise a selectable marker useful for identifying host cells into which the expression construct has been integrated and DNA sequences necessary for introduction of the construct into the plant in question (the latter depends on the DNA introduction method to be used).

The choice of regulatory sequences, such as promoter and terminator se
25 quences and optionally signal or transit sequences is determined, eg on the basis of
when, where and how the enzyme is desired to be expressed. For instance, the expression of the gene encoding the enzyme of the invention may be constitutive or inducible, or may be developmental, stage or tissue specific, and the gene product may
be targeted to a specific tissue or plant part such as seeds or leaves. Regulatory se
30 quences are eg described by Tague et al, Plant, Phys., 86, 506, 1988.

For constitutive expression the 35S-CaMV promoter may be used (Franck et al., 1980. Cell 21: 285-294). Organ-specific promoters may eg be a promoter from

storage sink tissues such as seeds, potato tubers, and fruits (Edwards & Coruzzi. 1990. Annu. Rev. Genet. 24: 275-303), or from metabolic sink tissues such as meristems (Ito et al., 1994. Plant Mol. Biol. 24: 863-878), a seed specific promoter such as the glutelin, prolamin, globulin or albumin promoter from rice (Wu et al., Plant and Cell 5 Physiology Vol. 39, No. 8 pp. 885-889 (1998)), a Vicia faba promoter from the legumin B4 and the unknown seed protein gene from Vicia faba described by Conrad U. et al, Journal of Plant Physiology Vol. 152, No. 6 pp. 708-711 (1998), a promotter from a seed oil body protein (Chen et al., Plant and cell physiology vol. 39, No. 9 pp. 935-941 (1998), the storage protein napA promoter from Brassica napus, or any other seed 10 specific promoter known in the art, eg as described in WO 91/14772. Furthermore, the promoter may be a leaf specific promoter such as the rbcs promoter from rice or tomato (Kyozuka et al., Plant Physiology Vol. 102, No. 3 pp. 991-1000 (1993), the chlorella virus adenine methyltransferase gene promoter (Mitra, A. and Higgins, DW. Plant Molecular Biology Vol. 26, No. 1 pp. 85-93 (1994), or the aldP gene promoter 15 from rice (Kagaya et al., Molecular and General Genetics Vol. 248, No. 6 pp. 668-674 (1995), or a wound inducible promoter such as the potato pin2 promoter (Xu et al, Plant Molecular Biology Vol. 22, No. 4 pp. 573-588 (1993).

A promoter enhancer element may be used to achieve higher expression of the enzyme in the plant. For instance, the promoter enhancer element may be an intron which is placed between the promoter and the nucleotide sequence encoding the enzyme. For instance, Xu et al. op cit disclose the use of the first intron of the rice actin 1 gene to enhance expression.

The selectable marker gene and any other parts of the expression construct may be chosen from those available in the art.

The DNA construct is incorporated into the plant genome according to conventional techniques known in the art, including *Agrobacterium*-mediated transformation, virus-mediated transformation, micro injection, particle bombardment, biolistic transformation, and electroporation (Gasser et al, Science, 244, 1293; Potrykus, Bio/Techn. 8, 535, 1990; Shimamoto et al, Nature, 338, 274, 1989).

Presently, *Agrobacterium tumefaciens* mediated gene transfer is the method of choice for generating transgenic dicots (for review Hooykas & Schilperoort, 1992. Plant Mol. Biol. 19: 15-38), however it can also be used for transforming monocots,

although other transformation methods are generally preferred for these plants. Presently, the method of choice for generating transgenic monocots is particle bombardment (microscopic gold or tungsten particles coated with the transforming DNA) of embryonic calli or developing embryos (Christou, 1992. Plant J. 2: 275-281; Shimamoto, 1994. Curr. Opin. Biotechnol. 5: 158-162; Vasil et al., 1992. Bio/Technology 10: 667-674). An alternative method for transformation of monocots is based on protoplast transformation as described by Omirulleh S, et al., Plant Molecular biology Vol. 21, No. 3 pp. 415-428 (1993).

Following transformation, the transformants having incorporated the expression construct are selected and regenerated into whole plants according to methods well-known in the art.

MATERIALS AND METHODS

Plasmids

pJSO026

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This is a *S. cerevisiae* expression plasmid described in WO 97/07205 and in J.S.Okkels, (1996) "A URA3-promoter deletion in a pYES vector increases the expression level of a fungal lipase in Saccharomyces cerevisiae. Recombinant DNA Biotechnology III: The Integration of Biological and Engineering Sciences, vol. 782 of the Annals of the New York Academy of Sciences).

20 pFuku83

This is a yeast and E. coli shuttle vector for expression of the H. insolens cutinase under the control of a TPI promoter, constructed from pJSO026.

Substrate

BETEB

Terephthalic acid bis(2-hydroxyethyl)ester dibenzoate is herein abbreviated as BETEB (benzoyl-ethylene-terephthalic-ethelene-benzoate). It was prepared from terephthalic acid bis (2-hydroxyethyl) ester and benzoic acid.

Lipase activity (LU)

A substrate for lipase is prepared by emulsifying tributyrin (glycerin tributyrate) using gum Arabic as emulsifier. The hydrolysis of tributyrin at 30 °C at pH 7 is followed in a pH-stat titration experiment. One unit of lipase activity (1 LU) equals the amount of enzyme capable of releasing 1 µmol butyric acid/min at the standard conditions.

Differential scanning calorimetry (DSC)

Sample and reference solutions are carefully degassed immediately prior to loading of samples into the calorimeter (reference: buffer without enzyme). Sample and reference solutions (approx. 0.5 ml) are thermally pre-equillibrated for 20 minutes at 5°C. The DSC scan is performed from 5 C to 95 C at a scan rate of approx. 90 K/hr. Denaturation temperatures are determined at an accuracy of approx. +/- 1 C. A VP-DSC from MicroCal Inc. is suitable for the experiments.

Methods

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15 PCR conditions

step 1: 94° C, 120 sec.

step 2: 94° C, 60 sec

step 3: 50° C, 60 sec

step 4: 72° C, 150 sec.

Go to step 2, 35 cycles

step 5: 72° C, 480 sec.

Step 6: 4° C, for ever

EXAMPLES

Example 1

Preparation of cutinase variants

A DNA sequence encoding *H. insolens* cutinase was obtained as described in US 5,827,719 (Novo Nordisk) and was found to have the DNA sequence shown in SEQ ID NO: 1 therein.

Variants were prepared by localized random mutagenesis and selection of positive clones by incubation at 60°C for 1 day on BETEB plates. The BETEB plates contained 200 ml/l of 500 mM glycine buffer (pH 8.5), 1.25 g/l of BETEB (dissolved in hot ethanol) and 20 g/l of agar.

Three-positive-variants (denoted JC013, JC014, JC025) were isolated, and their amino acid sequence was determined. They were found to have the following modifications, compared to the parent *H. insolens* cutinase:

JC013: A14P + E47K

JC014: E47K

JC025: E179Q

Example 2

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Site directed mutation

JC026 (E6Q, E47K, R51P) was prepared as follows:

A pair of PCR primers were designed so as to introduce amino acid substitutions, making use of the existed restriction enzyme sites nearby, as follows (an asterisk indicates an introduced mutation):

Upper primer: E6Q F

cgg cag ctg gga gcc atc c*ag aac

Pvu II

Lower primer: E47K,R51P

cgc cct_gga tcc aga tgt tcg* gga tgt ggg act t*aa ggc

BamH I

PCR was run using these primers and pFukuNL83 as a template under the PCR condition described above.

The obtained PCR fragment was purified by Clontech Spincolumn and digested with Pvu II and BamH I.

The resultant fragment was gel-purified and ligated to pFukuNL83 which had been digested with the same restriction enzyme sites.

Example 3

Thermostability of cutinase variants

Thermostability of cutinase variants was investigated by means of DSC (Differential Scanning Calorimetry) at pH 4.5 (50 mM acetate buffer) and pH 8.5 (50mM glycyl-glycine buffer). The thermal denaturation temperature, Td, was taken as the top of denaturation peak (major endothermic peak) in thermograms (Cp vs. T) obtained after heating of enzyme solutions at a constant programmed heating rate. The parent cutinase (NL83) was included for comparison. Results:

	pH 4.5	pH 8.5
JC013	-	70
JC014	•	70
JC015	65	70
JC026	64	71
JC029	66	73
JC038	64	71
JC039	66	73
IL83 (parent)	61	63

The results show improved thermostability in all cases. The improvement as seen to be 3-5° at pH 4.5, and 7-10° at pH 8.5.

Example 4

Hydrolysis of BETEB

The thermostability of *H*, insolens cutinase variants JC014 (E47K) and JC025 (E179Q) was measured by hydrolysis of BETEB at elevated temperature. The parent

		,16°	
55°C	33-014 1C014	"easured after the incuba	tion. The results are
60∘C ,	՝ (կ,		
65°C	* °Z	JC025	NL83 (parent)
70°C	^{او} 1	25 LU/ml	24 LU/ml
_	96	99 %	72 %
These results compared to the parent	6 %	83 %	33 %
compared to the	Clear	13 %	7 %
are parent	Citie 240"	6 %	7 %
compared to the parent	anuase w th	بدا	
		٧(ال	

Example 5 Hydrolysis of RETE

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The thermostability of cutinase was tested for comparison. The hydrolysis of BETEB at 60°C for 2 hours. The parent cutinase (denoted NL83) was varied. The results below are atture was carried out at the same conditions as 0 JC038

JC038

LU/ml

JC038

JC

10	0 %	My was tixed	at outcand the	cumase dosage
20	97 %	in the table	below.	
50	98 %	1C039	JC013	NL83 (parent)
100 98 % 88 %	0 %	0 %	0 %	
	99 %	9 %	6 %	
	99 %	74 %		
		94 %	93 %	15 %
		69 %	92 %	34 %

300	41 %
600	63 %
1200	82 %

The results show a much faster hydrolysis at 60°C with the variants than with the parent cutinase.

Example 6

5 Hydrolysis of c3ET

The thermostability of variants was measured by hydrolysis of c3ET at elevated temperature. Wild type (NL83) was tested for comparison. For each cutinase, the following mixture was incubated for 2 hours at various temperatures.

0.115mg c3ET (0.1ml of 2mM c3ET dissolved in HFIP was taken in reaction vessel. Solvent was removed under vacuum, then dried up at 70°C over night)

0.1ml 0.5M glycyl-glycine buffer (pH8.5)

0.1ml enzyme solution (approx. 600LU/ml)

0.8ml Milli Q water

After the incubation, 2ml of 1,1,1,3,3,3-Hexafluoro-2-propanol (HFIP) was added to each reaction mixture, then hydrolysis ratio was measured by HPLC. The results shown in Fig 3 clearly indicate the variants especially JC039 have improved thermostability compared to the parent cutinase.

Example 7

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Hydrolysis of c3ET on yarn

Similar experiment to the previous example was done using polyester yarn containing c3ET as by product. The following substrate mixture was preincubated at 60 or 65°C:

0.1g polyester yarn

0.2ml 0.5M glycyl-glycine buffer (pH8.5)

1.7ml Milli Q water

After preincubation, 0.1ml enzyme solution (approx. 1000 LU/ml) was added to each reaction vessel and incubated for 17 hours. Then 2ml HFIP was added and

left for 30 minutes to extract and hydrolyze c3ET sitting on the surface of the polyester yarn; then the hydrolysis ratio was measured. The results are shown in Fig. 4.

It is seen that the variants are more effective than the parent cutinase for hy-5 drolyzing c3ET on polyester yarn, particularly JC039. It is also seen that JC039 gives higher hydrolysis ratio at 65°C than 60°C.

Example 8

Treatment of yarn by variant JC039

Time courses of c3ET hydrolysis on polyester yarn at different temperature or dosage were examined. Time course at different temperatures is shown in Fig 5. It is seen that optimal temperature of JC039 is 65°C. At 70°C there is still about half of the activity left. Time course with increased enzyme dosage is shown in Fig 6. The curves at dosage 275 and 550 LU/ml are seen to be the same, indicating that the hydrolysis ratio reached to plateau between dosage of 100 to 275 LU/ml. Presumably 200LU/ml is enough.

CLAIMS

- 1. A variant of a parent fungal cutinase, which variant:
 - comprises substitution of one or more amino acid residues at a position which is located:
 - i) within 17 Å from the location of the N-terminal amino acid (as calculated from amino acid residues in a crystal structure), and/or
 - ii) within 20 positions from the N-terminal amino acid, and
 - b) is more thermostable than the parent cutinase.
- 2. The variant of the preceding claim which comprises substitution of one or more 10_amino acid residues at a position which is located:______
 - within 12 Å from the location of the N-terminal amino acid (as calculated from amino acid residues in a crystal structure), and/or
 - ii) within 15 positions from the N-terminal amino acid.
- 3. A variant of a parent fungal cutinase comprising substitution of one or more 15 amino acid residues which is located:
 - a) within 17 Å from the location of the N-terminal amino acid (as calculated from amino acid residues in a crystal structure), and/or
 - b) within 20 positions from the N-terminal amino acid,
- with the proviso that it is not a variant of the cutinase of *Fusarium solani pisi*having one of the substitutions R17, T18, T19V, D21N, I24E, Y38F, R40, G41A, S42, T43, E44, T45, G46, N47R, G49, T50, L51, P53, S54, A56C, S57, N58R, S61, A62E, K65A, D66S, G67D, W69Y, I70C, G74, G75, R78, Y119, G192, P193, D194R, A195, R196, G197V, or A199C (*Fusarium solani pisi* cutinase numbering).
- 4. A variant of a parent fungal cutinase comprising substitution of one or more amino acid residues which:
 - a) has a solvent accessible surface, and
 - b) is located:

- within 17 Å from the location of the N-terminal amino acid (as calculated from amino acid residues in a crystal structure), and/or
- ii) within 20 positions from the N-terminal amino acid,

with the proviso that it is not a variant of the cutinase of *Fusarium solani pisi* 5 having one of the substitutions T18, Y38F, R40, G41A, S42, T43, E44, T45, N47R, G49, T50, L51, P53, S54, A56C, A62E or G192 (*Fusarium solani pisi* cutinase numbering).

- 5. A variant of a parent fungal cutinase comprising substitution of one or more amino acid residues which is located:
- a) less than 12 Å from the location of the N-terminal amino group (as calculated from amino acid residues in a crystal structure), and/or
- b) within 15 positions from the N-terminal amino acid, with the proviso that the variant is not the cutinase of *Fusarium solani pisi* having one of the substitutions R17, T18, T19V, D21N, Y38F, R40, T45, G46, N47R, 15 G49, T50, L51, P53, S54, A56C, S57, N58R, K65A or I70C (*Fusarium solani pisi* cutinase numbering).
 - 6. The variant of any preceding claim wherein the parent cutinase is native to a filamentous fungus, preferably a strain of *Humicola* or *Fusarium*, preferably *H. insolens* or *F. solani pisi*, most preferably *H. insolens* strain DSM 1800.
- The variant of any preceding claim wherein the parent cutinase has an amino acid sequence which can be aligned with the cutinase of *H. insolens* strain DSM 1800.
- The variant of any preceding claim wherein the parent cutinase has an amino acid sequence which is at least 50 % homologous to the cutinase of *H. insolens* strain
 DSM 1800, preferably at least 70 % homologous, more preferably at least 80 % homologous.
 - 9. A variant of a parent fungal cutinase from Humicola insolens which comprises substitution of one or more amino acid residues located:

- a) within 17 Å from the location of the N-terminal amino acid (as calculated from amino acid residues in a crystal structure), and/or
- b) within 20 positions from the N-terminal amino acid.
- 10. The variant of the preceding claim which comprises substitution of one or more 5 amino acid residues located:
 - a) less than 12 Å from the location of the N-terminal amino group (as calculated from amino acid residues in a crystal structure), and/or
 - b) within 15 positions from the N-terminal amino acid
- 11. The variant of any preceding claim which comprises substitution of one or more amino acids having a solvent accessible surface.
 - 12. The variant of any preceding claim wherein one or more substitutions is substitution of a negatively charged amino acid with a neutral or positively charged amino acid or substitution of a neutral amino acid with a positively charged amino acid.
- 13. The variant of any preceding claim wherein one or more substitutions is sub15 stitution with a Pro residue.
- 14. The variant of any preceding claim wherein one or more substitutions is at a position corresponding to position E6, E10, A14, E47, R51 and/or E179 in the cutinase of *Humicola insolens* strain DSM 1800, preferably a substitution corresponding to E6Q, E10Q, A14P, E47K, R51P and/or E179Q (*H. insolens* cutinase numbering).
 - 15. The variant of any preceding claim which has one, two, three, four, five or six of said substitutions.
 - 16. The variant of any preceding claim which has substitutions corresponding to one of the following in the cutinase of *Humicola insolens* strain DSM 1800:
 - a) R51P
 - b) E6Q, L1381

- c) A14P, E47K
- d) E47K
- e) E179Q
- f) E6Q, E47K, R51P
- g) A14P, E47K, E179Q
- h) E47K, E179Q
- i) E47K, D63N
- j) E6Q, A14P, E47K, R51P, E179Q
- k) E6Q, E10Q, A14P, E47K, R51P, E179Q, or
- 10 I) Q1P, L2V, S11C, N15T, F24Y, L46I, E47K
 - 17. The variant of any preceding claim which has hydrolytic activity towards terephthalic acid esters, particularly towards cyclic tri(ethylene terephthalate) and/or Terephthalic acid bis(2-hydroxyethyl)ester dibenzoate (BETEB).
- 18. The variant of any preceding claim which has a denaturation temperature which is at least 5° higher than the parent cutinase, preferably measured at pH 8.5
 - 19. A DNA sequence encoding the variant of any preceding claim.
 - 20. A vector comprising the DNA sequence of the preceding claim.
 - 21. A transformed host cell harboring the DNA sequence of claim 19 or the vector of claim 20.
- 20 22. A method of producing the variant of any of claims 1-18 comprising
 - a) cultivating the cell of claim 21 so as to express and preferably secrete the variant, and
 - b) recovering the variant.
 - 23. A method of constructing a cutinase variant, which method comprises:
- 25 a) selecting a parent fungal cutinase,

- 1.000-DK
 - b) identifying one or more amino acid residues in the parent cutinase at positions which are:
 - within 17 Å from the location of the N-terminal amino acid (as calculated from amino acid residues in a crystal structure), and/or
 - ii) within 20 positions from the N-terminal amino acid, and
 - c) making alterations each of which is an insertion, a deletion or a substitution of the amino acid residue,
 - optionally, making alterations each of which is an insertion, a deletion or a substitution of an amino acid residue at one or more positions other than b),
 - e) preparing the variant resulting from steps b-d,
 - f) testing the thermostability of the variant,
 - g) optionally repeating steps b-f, and
 - h) selecting a variant having higher thermostability than the parent cutinase.

A method of producing a cutinase variant, which method comprises:

- a) selecting a parent fungal cutinase,
- b) identifying one or more amino acid residues in the parent cutinase at positions which are:
 - i) within 17 Å from the location of the N-terminal amino acid (as calculated from amino acid residues in a crystal structure), and/or
 - ii) within 20 positions from the N-terminal amino acid, and
- making alterations each of which is an insertion, a deletion or a substitution of the amino acid residue,
- optionally, making alterations each of which is an insertion, a deletion or a substitution of an amino acid residue at one or more positions other than b).
- preparing the variant resulting from steps b-d,
- testing the thermostability of the variant,
- のptionally repeating steps b-f,

- h) selecting a variant having higher thermostability than the parent cutinase, and
- i) producing the variant to obtain the cutinase variant.
- 25. A process for enzymatic hydrolysis of a cyclic oligomer of poly(ethylene tere-5 phthalate), which process comprises treating the cyclic oligomer with a variant of a parent fungal cutinase, which variant comprises substitution of one or more amino acid residues at a position which is located:
 - i) within 17 Å from the location of the N-terminal amino acid (as calculated from amino acid residues in a crystal structure), and/or
 - ii) within 20 positions from the N-terminal amino acid.
 - 26. The process of the preceding claim, in which the cyclic oligomer is cyclic tri(ethylene terephthalate).
 - 27. The process of claim 25 or 26 wherein the treatment is done at 60-75°C, preferably at 65-70°C.
- 15 28. The process of any of claims 25-27 wherein the cyclic oligomer is present in and on the fibers of a polyester containing fabric or yarn.
 - 29. The process of any of claims 25-28 which further comprises subsequently rinsing the fabric or yarn, preferably rinsing with an aqueous solution having a pH in the range of from about pH 7 to about pH 11.
- 20 30. A detergent composition comprising a surfactant and the variant of any of claims 1-18.
 - 31. A method for detecting cutinase activity in a sample, comprising incubating the sample with terephthalic acid bis(2-hydroxyethyl)ester dibenzoate and detecting hydrolysis of said ester.

Fig. 1 3D structure of cutinase from Humicola insolens MOTA N GLY A 24.424 -7.935 18.390 1 3 1.00 46.73 MOTA 2 CA GLY A 3 23.848 -8.994 17.546 1.00 42.29 ATOM 3 C GLY A 24.396 -10.112 3 16.727 1.00 37.35 MOTA 4 O GLY A 25.347 -10.913 16.728 1.00 35.38 MOTA 5 N ALA A 23.664 -10.625 15.797 1.00 34.53 **MOTA** 6 CA ALA A 23.051 -10.874 14.555 1.00 30.95 MOTA 7 C ALA A 21.574 -11.246 14.920 1.00 28.33 10 ATOM 8 0 ALA A 20.677 -10.499 14.446 1.00 22.94 ATOM 9 CB ALA A 23.574 -11.780 13.556 1.00 26.92 MOTA 10 N ILE A 5 21.583 -12.058 16.043 1.00 26.48 MOTA 11 CA ILE A 5 20.281 -12.289 16.637 1.00 25.65 MOTA С ILE A 12 5 20.316 -12.151 18.118 1.00 22.40 **15 ATOM** 13 0 ILE A 5 21.060 -12.888 18.717 1.00 24.74 MOTA CB ILE A 5 19.724 -13.683 14 16.524 1.00 26.04 ATOM 15 CG1 ILE A 5 19.852 -13.927 15.050 1.00 29.85 18.374 -13.558 **ATOM** CG2 ILE A 16 5 17.159 1.00 20.48 **ATOM** 17 CD1 ILE A 14.709 1.00 27.96 5 19.066 -15.133 20 ATOM 18 N GLU A 6 19.461 -11.377 18.668 1.00 20.52 MOTA 19 CA GLU A 19.207 -11.015 6 20.040 1.00 17.94 ATOM 20 C. GLU A 6 17.711 -11.027 20.432 1.00 17.76 ATOM GLU A 21 0 16.931 -10.165 19.990 1.00 17.60 MOTA 22 CB GLU A 19.809 -9.614 20.199 1.00 14.22 25 атом 23 CG GLU A 6 21.232 -9.374 20.385 1.00 16.71 CD GLU A MOTA 24 6 22.148 -10.387 21.030 1.00 34.47 MOTA 25 OE1 GLU A 21.634 -11.347 6 21.693 1.00 49.57 ATOM 26 OE2 GLU A 6 23.410 -10.310 20.975 1.00 37.43 ATOM 27 N ASN A 7 17.375 -11.895 21.333 1.00 21.67 30 ATOM 28 CA ASN A 7 16.070 -11.854 21.846 1.00 24.04 MOTA 29 С ASN A 15.927 -11.488 23.238 1.00 22.08 MOTA 30 0 ASN A 7 15.098 -12.179 23.820 1.00 24.00 ATOM 31 CB ASN A 7 15.468 -13.307 21.820 1.00 25.06 MOTA CG 7 32 ASN A 15.039 -13.160 20.341 1.00 38.52 35 ATOM OD1 ASN A 33 15.519 -14.147 19.759 1.00 48.45 MOTA 34 ND2 ASN A 7 14.318 -12.081 19.968 1.00 36.89 ATOM 35 N GLY A 8 16.671 -10.813 23.926 1.00 23.56 MOTA 36 CA GLY A 8 16.654 -10.628 25.363 1.00 23.69 **MOTA** 37 C GLY A 8 15.366 -10.247 25.984 1.00 22.72 40 ATOM 38 0 GLY A 8 14.967 -10.939 26.867 1.00 32.25 **ATOM** 39 N LEU A 9 14.785 -9.144 25.755 1.00 23.61 MOTA 40 CA LEU A 9 13.470 -8.753 26.033 1.00 23.73 MOTA 41 C LEU A 9 12.559 -9.961 25.782 1.00 25.93 ATOM 42 0 LEU A 9 11.494 ~10.054 26.480 1.00 30.47 45 _{ATOM} CB 43 LEU A 9 12.971 -7.621 25.105 1.00 5.84 ATOM CG LEU A 44 9 11.556 -7.227 25.470 1.00 23.25 ATOM 45 CD1 LEU A 11.422 -6.765 9 26.968 1.00 20.21 MOTA 46 CD2 LEU A 11.009 -6.071 9 24.714 1.00 17.64 ATOM 47 N GLU A 10 12.775 -10.786 24.773 1.00 29.56 ŠÕ ATOM

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MOTA

ATOM

CA

GLU A

GLU A

GLU A

10

10

10

11.635 -11.681

11.640 -12.872

10.600 -13.159

24.484

1.00 33.93

25.412 1.00 32.18

25.996 1.00 36.67

CB GLU A 10 11.513 -11.996 23.012 1.00 40.97 MOTA ATOM GLU A 10 10.054 -12.303 22.745 1.00 51.96 53 CD GLU A 10 9.570 -11.711 21.437 1.00 54.08 MOTA 54 OE1 GLU A 10 10.488 -11.440 20.635 1.00 48.22 **ATOM** 1.00 52.39 21.471 5 ATOM 55 OE2 GLU A 10 8.323 -11.643 12.822 -13.334 25.688 1.00 29.58 56 N SER A 11 ATOM 26.645 1.00 35.25 12.993 -14.455 57 ÇA SER A 11 ATOM 13.403 -14.012 28.047 1.00 39.86 MOTA 58 С SER A 11 28.919 1.00 43.72 MOTA 59 0 SER A 11 13.688 -14.790 14.053 -15.364 25.983 1.00 33.73 CB SER A 11 10 ATOM 60 1.00 46.98 OG SER A 11 15.275 -14.620 25.928 MOTA 61 28.456 1.00 41.40 13.467 -12.802 ATOM 62 N GLY A 12 13.841 -12.332 CA GLY A 12 29.752 1.00 45.34 MOTA 63 64 C GLY A 12 12.673 -12.562 30.694 1.00 47.62 MOTA 65 0 GLY A 12 11.485 -12.335 30.335 1.00 50.76 **15 ATOM** 66 N SER A 13 12.969 -12.900 31.936 1.00 48.09 ATOM MOTA 67 CA SER A 13 11.974 -13.158 32.995 1.00 45.26 11.509 -11.933 33.772 1.00 39.53 MOTA 68 C SER A 13 33.992 1.00 36.30 12.563 -11.204 MOTA 69 0 SER A 13 -12.708--14.006-34.101-- 1.00-51.20--20- ATOM-70 --CB---SER -A- -13-SER A 13 12.006 -13.947 35.338 1.00 57.14 MOTA 71 OG ALA A 14 10.256 -11.785 34.214 1.00 35.22 MOTA 72 N ALA A 14 10.068 -10.530 34.964 1.00 34.78 CA MOTA 73 10.574 -10.620 36.417 1.00 37.51 C ALA A 14 MOTA 74 25 атом 75 0 ALA A 14 10.809 -9.584 37.113 1.00 38.41 8.714 -9.915 34.903 1.00 32.71 ATOM 76 CB ALA A 14 77 N ASN A 15 11.039 -11.834 36.737 1.00 38.85 MOTA 11.715 -12.086 37.963 1.00 43.49 MOTA 78 CA ASN A 15 С ASN A 15 13.073 -11.411 37.953 1.00 46.45 MOTA 79 13.453 -11.022 39.022 1.00 52.50 30 ATOM 80 0 ASN A 15 12.088 -13.533 38.207 1.00 53.08 **ATOM** 81 CB ASN A 15 10.772 -14.226 38.553 1.00 71.86 CG ASN A 15 MOTA 82 38.998 1.00 71.73 OD1 ASN A 15 9.837 -13.535 ATOM 83 ND2 ASN A 15 10.866 -15.523 38.267 1.00 77.71 MOTA 84 **35 ATOM** ALA A 16 85 N 13.712 -11.305 36.812 1.00 46.73 36.743 ATOM 86 CA ALA A 16 14.915 -10.470 1.00 41.22 MOTA 87 C ALA A 16 15.031 -9.286 35.798 1.00 36.70 MOTA 88 0 ALA A 16 16.027 -9.254 35.075 1.00 37.67 15.903 -11.545 36.301 1.00 41.80 MOTA 89 CB ALA A 16 **40** ATOM N CYS A 14.300 -8.227 35.843 1.00 30.62 90 17 CYS A 14.614 -7.093 34.997 1.00 31,78 **ATOM** 91 CA 17 С CYS A 17 16.024 -6.579 35.149 1.00 32.94 MOTA 92 0 16.744 -6.850 36.113 1.00 39.10 MOTA 93 CYS A 17 MOTA CB CYS A 17 13.679 -5.881 35.138 1.00 28.00 94 **45** ATOM -6.583 34.858 1.00 24.72 95 SG CYS A 17 12.048 16.529 -5.910 34.092 1.00 30.49 96 N PRO A 18 **ATOM** -5.626 33.971 1.00 22.04 CA PRO A 18 17.994 **ATOM** 97 18.178 -4.138 34.241 1.00 20.15 MOTA С PRO A 18 98 **ATOM** 99 0 PRO A 18 17.085 -3.459 34.370 1.00 17.83 50 ATOM 1.00 19.20 PRO A 18 18.353 -6.003 32.559 100 CB PRO A 18 17.044 -6.595 32.101 1.00 20.16 ATOM 101 CG 32.792 1.00 24.35 15.903 -5.936 ATOM 102 PRO A 18 19.428 -3.652 34.011 1.00 14.85 MOTA 103 ASP A 19

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ASP A 19 CA 19.451 -2.168 34.226 1.00 16.59 104 MOTA 18.739 -1.367 33.156 С ASP A 19 1.00 20.42 105 ATOM 106 0 ASP A 19 18.311 -0.242 33.430 1.00 23.84 **ATOM ATOM** 107 CB ASP A 19 20.896 -1.818 34.485 -2.389 35.793 5 ATOM ASP A 19 21.433 108 CG -3.549 36.297 OD1 ASP A 19 21.162 **ATOM** 109 22.251 -1.719 36.543 1.00 54.02 OD2 ASP A 19 **ATOM** 110 MOTA 111 N ALA A 20 18.646 -1.780 31.895 1.00 20.18 1.00 17.43 ALA A 20 18.066 -1.036 30.809 MOTA 112 CA 29.703 1.00 16.06 ALA A 20 17.713 -2.087 10 ATOM 113 C -3.172 29.860 1.00 9.45 ALA A 20 18.334 MOTA 114 0 ALA A 20 18.975 -0.04B 30.100 1.00 12.07 **ATOM** 115 CB 28.829 1.00 8.47 **ATOM** 116 N ILE A 21 16.814 -1.602 -2.583 27.753 1.00 9.23 16.657 MOTA 117 CA ILE A 21 -1.745 26.486 1.00 14.77 16.952 **15 ATOM** 118 С ILE A 21 -0.473 26.403 1.00 12.01 ILE A 21 16.681 ATOM 119 0 -2.984 27.837 1.00 16.28 CB ILE A 21 15.208 **ATOM** 120 -3.898 28.956 1.00 15.55 CG1 ILE A 21 14.851 ATOM 121 14.689 -3.671 26.514 1.00 13.71 CG2 ILE A 21 ATOM 122 -3.879 CD1 ILE A 21 _ 13.401 29.372 1.00 6.12 20 ATOM 123 1.00 12.24 124 N LEU A 22 17.432 -2.451 25.391 MOTA -1.774 24.087 1.00 11.27 ATOM 125 CA LEU A 22 17.665 16.849 -2.517 23.038 1.00 14.60 MOTA 126 С LEU A 22 16.908 -3.781 22.850 1.00 9.78 ATOM 127 0 LEU A 22 25 ATOM LEU A 22 19.087 -1.865 23.693 1.00 10.96 128 CB 1.00 10.32 -1.543 22.257 MOTA 129 CG LEU A 22 19.493 1.00 4.72 -0.081 21.900 19.311 MOTA 130 CD1 LEU A 22 -1.842 22.156 1.00 7.42 20.990 ATOM 131 CD2 LEU A 22 ILE A 23 16.038 -1.815 22.242 1.00 15.13 MOTA 132 N **30** ATOM 15.298 -2.459 21.115 1.00 18.06 133 CA ILE A 23 ILE A 23 -1.771 19.901 1.00 17.42 15.916 ATOM 134 С 16.117. -0.519 19.795 1.00 19.31 0 ILE A 23 MOTA 135 CB ILE A 23 13.820 -2.194 21.392 1.00 18.16 MOTA 136 22.447 13.208 -3.076 1.00 14.23 MOTA 137 CG1 ILE A 23 12.787 -2.167 20.247 1.00 13.19 35 ATOM CG2 ILE A 23 138 12.142 -2.065 22.976 1.00 20.41 139 CD1 ILE A 23 **ATOM** -2.548 18.940 **MOTA** 140 N PHE A 24 16.218 1.00 14.59 16.859 -2.159 17.671 1.00 11.72 PHE A 24 ATOM 141 CA 1.00 7.25 16.347 -2.719 16.353 C PHE A 24 MOTA 142 1.00 3.47 **40** ATOM 0 PHE A 24 16.095 -3.998 16.161 143 18.195 -2.855 17.658 1.00 12:61 MOTA 144 CB PHE A 24 19.015 -2.150 16.716 1.00 10.72 **ATOM** 145 CG PHE A 24 1.00 13.08 CD1 PHE A 24 19.457 -0.844 16.913 ATOM 146 CD2 PHE A 24 19.325 -2.852 15.558 1.00 6.61 MOTA 147 45 ATOM 148 CE1 PHE A 24 20.232 -0.187 15.983 1.00 4.86 1.00 7.61 -2.218 14.545 MOTA 149 CE2 PHE A 24 20.061 14.804 1.00 8.78 -0.823 ATOM 150 CZ PHE A 24 20.550 -1.700 15.449 1.00 6.32 16.037 **ATOM** 151 N ALA A 25 15.662 -2.158 1.00 14.068 MOTA 152 CA ALA A 25 50 ATOM 13.055 1.00 8.59 -1.976 153 С ALA A 25 16.851 17.518 -1.000 1.00 5.95 13.133 25 **ATOM** 154 0 ALA A 14.488 -1.402 13.562 1.00 25 MOTA 155 CB ALA A ARG A 26 17.174 -3.032 12.325 1.00 **ATOM** 156 N

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Professional Broad Benediction

الرواف والمتعارض والمتعارض

MOTA 157 CA ARG A 26 18.134 -3.278 11.277 1.00 4.04 MOTA 158 С ARG A 26 17.691 -2.694 9.894 7.67 MOTA 159 0 ARG A 26 16.527 -2.361 9.525 1.00 9.36 **ATOM** 160 CB ARG A 26 18.581 -4.659 10.756 1.00 17.705 ATOM 161 CG ARG A 26 -5.741 10.439 1.00 **ATOM** 162 CD ARG A 26 18.069 -7.224 10.382 1.00 ATOM 17.000 163 NE ARG A 26 -8.053 9.708 1.00 9.04 MOTA 164 CZARG A 26 15.724 -8.206 9.912 1.00 7.06 MOTA 165 NH1 ARG A 26 15.085 -7.535 10.895 1.00 22.93 **10 ATOM** 166 NH2 ARG A 26 14.809 -8.825 9.346 1.00 ATOM 167 N GLY A 27 18.761 -2.539 9.092 1.00 MOTA 168 CA GLY A 27 18.537 -1.888 7.782 1.00 5.34 ATOM 169 C GLY A 27 18.063 -2.896 6.862 1.00 4.70 170 **ATOM** 0 GLY A 27 18.155 -4.139 7.075 1.00 13.14 171 **15 ATOM** N SER A 17.562 -2.612 5.765 28 1.00 11.82 172 CA ATOM SER A 17.108 -3.325 4.615 28 1.00 14.72 ATOM 173 C SER A 28 18.214 -4.327 4.142 1.00 7.74 ATOM 174 O SER A 28 19.286 -3.973 4.083 1.00 6.71 MOTA 175 CB SER A -2.352 3.538 28 16.460 1.00 6.38 20 ATOM 176 OG SER A 28 16.819 -0.978 3.833 1.00 28.10 177 ATOM N THR A 29 17.942 -5.634 4.241 1.00 4.79 ATOM 178 CA THR A 29 18.562 -6.763 3.914 1.00 B.71 ATOM 179 C THR A 29 19.500 -7.271 4.985 1.00 14.00 **ATOM** 180 0 THR A 29 20.162 -8.326 4.713 1.00 17.68 25 ATOM 181 CB THR A 29 19.454 -6.680 2.617 1.00 14.90 **ATOM** 182 OG1 THR A 29 20.736 -6.066 2.595 1.00 14.00 ATOM 183 CG2 THR A -5.888 29 18.785 1.561 1.00 15.59 MOTA 184 -6.599 N GLU A 30 19.740 6.105 1.00 14.52 MOTA 185 CA GLU A 30 20.677 -7.266 7.056 1.00 14.10 30 ATOM 186 С GLU A 30 20.092 -8.513 7.647 1.00 13.07 ATOM 187 0 GLU A 30 18.916 -8.726 7.705 1.00 19.98 MOTA 188 CB GLU A 21.228 - -6.371 8.072 30 1.00 15.45 MOTA 189 CG GLU A 30 21.166 -4.945 7.709 1.00 8.37 ATOM 190 CD GLU A 30 22.073 -4.143 8.637 1.00 23.08 35 ATOM OE1 GLU A ~3.328 9.284 191 30 21.395 1.00 19.26 ATOM OE2 GLU A -4.327 8.712 192 30 23.317 1.00 19.71 MOTA 193 N PRO A 31 20.875 ~9.479 7.918 1.00 13.09 MOTA 194 CA PRO A 31 20.477 -10.818 8.402 1.00 14.56 MOTA 195 C PRO A 20.167 -10.698 31 9.895 1.00 18.27 40 атом 196 0 PRO A 31 20.148 -9.636 10.392 1.00 20.45 ATOM 197 CB PRO A 31 21.690 -11.692 8.215 1.00 10.95 **ATOM** 198 CG PRO A 31 22.790 -10.664 8.455 1.00 11.24 MOTA 199 CD PRO A 31 22.350 -9.316 7.864 1.00 13.71 MOTA 200 N GLY A 19.612 -11.689 10.472 1.00 18.99 32 **45** атом 201 CA GLY A 19.205 -11.774 11.816 1.00 13.53 32 ATOM 202 C GLY A 18.133 -10.808 12.188 1.00 16.62 32 ATOM GLY A 203 0 17.345 -10.294 11.411 1.00 17.01 32 MOTA 204 N ASN A 18.055 -10.528 13.468 1.00 16.15 33 **ATOM** 205 CA ASN A 33 17.290 -9.346 13.823 1.00 14.74 50 ATOM 18.294 206 C ASN A 33 -8.273 14.230 1.00 15.46 -7.184 **ATOM** 207 0 ASN A 17.774 14.575 33 1.00 15.90 14.867 **ATOM** 208 CB ASN A 16.241 -9.663 33 1.00 17.42 MOTA 209 CG ASN A 33 16.827 -10.201 16.127 1.00 17.97

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MOTA 210 OD1 ASN A 33 16.112 -10.395 17.089 1.00 19.05 **ATOM** 211 ND2 ASN A 33 18.074 -10.460 16.112 1.00 13.29 ATOM 212 N MET A 34 19.633 -8.378 14.282 1.00 14.22 ATOM 213 CA MET A 34 20.282 -7.171 14.751 1.00 12.97 5 ATOM 214 C MET A 34 21.142 -6.663 13.611 1.00 19.02 ATOM 215 0 MET A 34 21.654 -5.512 13.713 1.00 26.04 -7.329 **ATOM** CB 216 MET A 34 21.202 15.859 1.00 13.39 MET A MOTA 217 CG -7.713 34 20.579 17.163 1.00 9.02 MOTA 218 SD MET A -6.316 34 20.175 18.069 1.00 9.13 **10 ATOM** 219 CE MET A 18.095 34 21.481 -5.121 1.00 4.11 MOTA 220 N GLY A -7.446 35 21.259 12.550 1.00 19.99 ATOM 221 CA GLY A 35 22.071 -7.135 11,418 1.00 14.30 MOTA 222 Ç GLY A 35 23.511 -7.340 11.764 1.00 17.58 MOTA 223 O GLY A 35 23.965 -7.724 12.842 1.00 12.78 **15** ATOM 224 N ILE A 36 24.450 -6.839 10.950 1.00 20.63 **ATOM** 225 CA ILE A 36 25.833 -7.029 11.277 1.00 17.71 ATOM 226 С ILE A 36 26.609 -5.714 11.280 1.00 16.15 MOTA 227 0 ILE A 36 27.865 -5.618 11.662 1.00 20.30 ATOM 228 CB ILE A 36 26.412 -8.070 10.327 1.00 30.19 20 ATOM CG1 ILE A 8.959 229 26.088 -7.448 36 1.00 31.16 MOTA 230 CG2 ILE A 25.944 10.543 36 -9.490 1.00 15.68 ATOM 231 CD1 ILE A 36 26.922 -8.149 7.958 1.00 34.10 **ATOM** 232 N THR A 37 25.905 -4.589 11.040 1.00 13.00 MOTA 233 CA THR A 37 26.825 -3.396 11.141 1.00 9.67 **25** ATOM THR A 234 C 37 26.587 -2.513 12.350 1.00 15.44 **ATOM** 235 0 THR A 37 27.040 -3.055 13.410 1.00 20.20 MOTA 236 CB THR A 37 26.592 -2.679 9.818 1.00 14.13 MOTA 237 OG1 THR A 37 25.241 -2.212 9.503 1.00 22.62 MOTA 238 CG2 THR A 37 26,949 -3.739 8.800 1.00 2.29 30 ATOM 25.733 239 N VAL A 38 -1.493 12.249 1.00 11.92 ATOM 240 VAL A CA 38 25.237 -0.800 13.411 1.00 15,22 MOTA 241 С VAL A 24.588 -1.455 38 14.612 1.00 14.68 MOTA 242 0 VAL A 38 24.906 -1.185 15.733 1.00 15.89 MOTA 243 VAL A CB 38 24.124 0.180 12.855 1.00 14.13 35 атом 244 CG1 VAL A 38 23.663 0.897 1.00 13.55 14.167 MOTA 245 CG2 VAL A 24.570 1.025 38 11.670 1.00 6.75 ATOM N 246 GLY A 39 23.745 -2.410 14.677 1.00 14.24 MOTA 247 CA GLY A 39 23.135 -3.151 15.746 1.00 11.03 MOTA 248 С GLY A 39 24.096 -3.586 16.791 1.00 13.34 40 атом 249 0 GLY A 39 24.131 -3.181 17.934 1.00 15.13 MOTA 250 N PRO A 40 25.067 -4.340 16.352 1.00 14:70 MOTA 251 CA PRO A 40 26.094 -5.025 17.171 1.00 13.44 MOTA 252 C PRO A 27.010 -3.909 17.589 40 1.00 11.81 MOTA 253 0 PRO A 40 27.346 -3.871 18.764 1.00 12.79 45 ATOM 254 CB PRO A 40 26.723 -6.111 16.279 1.00 8.43 ATOM 255 CG PRO A 40 25.873 -6.243 14.950 1.00 4.84 MOTA CD PRO A -4.902 256 40 25.198 14.995 1.00 12.36 MOTA 1.00 7.41 257 N -2.979 16.695 ALA A 41 27.226 MOTA 258 CA ALA A 28.066 -1.962 17.278 41 1.00 11.03 50 ATOM C -1.206 259 ALA A 41 27.378 18.439 1.00 14.87 MOTA 0 -0.503 260 ALA A 41 28.028 19.274 1.00 14.26 **ATOM** -0.905 261 CB ALA A 41 28.579 1.00 7.17 16.313 MOTA 262 N LEU A 42 26.135 -0.811 18.237 1.00 11.87

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CA LEU A 42
                                     25.487
                                             -0.048 19.300
  MOTA
           263
                                                              1.00 12.36
                 С
                     LEU A
                                             -0.856
           264
                            42
                                     25.337
                                                      20.624
  MOTA
                                                              1.00 11.94
                                             -0.397
  ATOM
           265
                 0
                     LEU A
                            42
                                     25.423
                                                      21.730
                                                              1.00 8.33
                                     24.036
                                              0.168
                                                      18.811
           266
                 CB
                     LEU A
                            42
                                                              1.00 13.24
   ATOM
                     LEU A
                             42
                                     23.272
                                              1.160
                                                      19.676
                                                              1.00
                                                                     6.90
  ATOM
           267
                 CG
           268
                 CD1
                     LEU A
                             42
                                     24.108
                                              2.419
                                                      19.962
                                                              1.00
                                                                     6.62
   ATOM
                                     21.991
                                              1.580
                                                      18.943
   MOTA
           269
                 CD2
                     LEU A
                             42
                                                               1.00
   MOTA
           270
                 N
                     ALA A
                             43
                                     24.905
                                             -2.095
                                                      20.482
                                                               1.00 10.88
   MOTA
           271
                                     24.761
                                             -3.027
                                                      21.553
                                                              1.00 12.37
                 CA
                     ALA A
                             43
10 ATOM
           272
                 C
                     ALA A
                                     26.106
                                             -3.136
                                                      22.252
                                                              1.00 15.45
                             43
   ATOM
           273
                 0
                     ALA A
                                     25.958
                                             -2.743
                                                      23.433
                                                              1.00 20.80
                             43
                                             -4.324
                                                      21.002
   ATOM
           274
                 CB
                     ALA A
                             43
                                     24.148
                                                              1.00 9.60
                                             -3.440
                                     27.263
                                                      21.636
                                                              1.00 16.91
   MOTA
           275
                 N
                     ASN A
                             44
                                     28.454
                                             -3.434
                                                      22.439
                                                              1.00 20.33
   MOTA
           276
                 CA
                     ASN A
                             44
                                     28.717
                                             -2.044
                                                      23.113
                                                              1.00 17.66
15 ATOM
           277
                 С
                     ASN A
                             44
           278
                 O
                     ASN A
                             44
                                     29.019
                                             -1.991
                                                      24.301
                                                              1.00 17.06
   ATOM
                                                      21.625
                                             -3.695
   MOTA
           279
                 CB
                     ASN A
                                     29.756
                             44
                                     29.564
                                             -5.115
                                                     21.138
                                                              1.00 58.23
   ATOM
           280
                 CG
                     ASN A
                             44
   MOTA
            281
                 OD1 ASN A
                                     30.013
                                             -5.403
                                                     20.034
                                                              1.00 79.77
                                     28.908 -5.945 21.921 1.00 70.10
20-- атом-
           282
                 ND2 ASN A 44
                                     28.682 -0.988 22.297
                                                              1.00 14.39
   MOTA
            283
                 N
                     GLY A 45
                                     29.015
                                               0.221 22.976
                                                              1.00 11.65
   MOTA
            284
                 CA
                     GLY A
                            45
                                     28.175
                                               0.255
                                                      24.234
                                                               1.00 14.30
   MOTA
            285
                 C
                     GLY A
                             45
                                     28.529
                                               0.582
                                                      25.385
                                                               1.00 10.77
   MOTA
            286
                 O
                     GLY A
                             45
25 атом
            287
                 N
                     LEU A
                                     26.861
                                               0.099
                                                      24.065
                                                               1.00 16.88
                             46
   MOTA
            288
                 CA
                     LEU A
                             46
                                     25.968
                                               0.248
                                                      25.207
                                                               1.00 16.29
                      LEU A
                                      26.395
                                              -0.651
                                                      26.346
                                                               1.00 13.48
   MOTA
            289
                 C
                             46
                                                      27.462
   MOTA
            290
                 0
                      LEU A
                             46
                                      26.579
                                              -0.325
                                                               1.00 7.75
                                      24.608
                                              -0.243
                                                       24.847
                                                               1.00 19.46
   MOTA
            291
                 CB
                     LEU A
                             46
30 ATOM
                                                       25.664
            292
                 CG
                     LEU A
                             46
                                      23.642
                                               0.551
                                                               1.00 13.97
                                      24.089
                                               1.994
                                                       25.563
                                                               1.00 13.99
   MOTA
            293
                 CD1 LEU A
                             46
   MOTA
                 CD2 LEU A
                                      22.275
                                               0.465
                                                       25.038
                                                               1.00 32.18
            294
                             46
   MOTA
            295
                 N
                      GLU A
                                      26.523
                                              -1.890
                                                       25.882
                                                               1.00 15.90
                                                       26.909
            296
                 CA
                      GLU A
                             47
                                      26.910
                                              -2.886
                                                               1.00 24.03
   MOTA
35 ATOM
                                                       27.702
                                              -2.500
                                                               1.00 24.14
            297
                 С
                      GLU A
                             47
                                      28.140
            298
                             47
                                      28.722
                                              -3.203
                                                       28.500
                                                               1.00 27.24
   MOTA
                 0
                      GLU A
                                              -4.206
                                                       26.204
                                                               1.00 33.33
    MOTA
            299
                 CB
                      GLU A
                             47
                                      27.147
                                      27.386
                                              -5.254
                                                       27.245
                                                               1.00 51.29
    ATOM
            300
                 CG
                      GLU A
                             47
                                              -6.560
                                                       26.524
                                                               1.00 68.40
    MOTA
            301
                 CD
                      GLU A
                             47
                                      27.661
 40 ATOM
            302
                 OE1 GLU A
                             47
                                      26.741
                                              -7.007
                                                       25.777
                                                               1.00 66.37
    ATOM
            303
                 OE2 GLU A
                             47
                                      28.856
                                              -6.921
                                                       26.830
                                                               1.00 78'.70
                                              -1.626
                                                       27.215
                                                               1.00 27.50
    ATOM
            304
                 N
                      SER A
                              48
                                      28.992
                                      30.331
                                              -1.518
                                                       27.789
                                                               1.00 25.23
    ATOM
            305
                 CA
                      SER A
                             48
                                                       28.926
    ATOM
            306
                 C
                      SER A
                              48
                                      30.108
                                              -0.555
                                                               1.00 26.91
 45 ATOM
                                                       29.462
                                                               1.00 33.39
                                              -0.058
            307
                 0
                      SER A
                             48
                                      31.124
                                              -0.990
                                                       26.621
                                                               1.00 21.90
                                      31.116
    MOTA
            308
                 CB
                      SER A
                              48
                                      31.294
                                                0.422
                                                       26.483
    MOTA
                 OG
                      SER A
                              48
            309
                                                       28.995
                                                                1.00 25.04
    MOTA
                 N
                      HIS A
                              49
                                      28.826
                                               -0.101
            310
                                                       29.956
                                                                1.00 19.72
    ATOM
                      HIS A
                              49
                                      28.542
                                                0.955
            311
                 CA
 50 ATOM
                                                       30.950
                                                                1.00 22.55
                      HIS A
                              49
                                      27.480
                                                0.461
                  C
            312
                                      27.186
                                                1.089
                                                       31.898
                                                               1.00 27.93
    MOTA
                      HIS A
                              49
            313
                  0
    ATOM
             314
                  CB
                      HIS A
                              49
                                      28.094
                                                2.197
                                                       29.463
                                                               1.00 16.13
                                                       28.520
                                                                1.00 39.79
                                                3.036
    MOTA
                  CG
                      HIS A
                             49
                                      28.806
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्राप्ताः । अस्य अस्ति । स्वारं क्रिकेट । स्

5677-000, SLK, 1998-12-04

A CARLO DE LA COLONIA DE LA CO

भागमाना है। असे के क्षेत्र के कि

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MOTA
                ND1 HIS A
                                     29.564
                                              4.058
           316
                            49
                                                     28.953
                                                             1.00 45.66
  MOTA
           317
                CD2 HIS A
                            49
                                     28.776
                                              3.070
                                                      27.197
                                                              1.00 46.91
  MOTA
           318
                CE1 HIS A
                            49
                                     30.028
                                              4.750
                                                      27.979
                                                              1.00 45.87
  MOTA
           319
                NE2 HIS A
                            49
                                     29.544
                                              4.139
                                                      26.934
                                                              1.00 50.84
                                             -0.703
                                                      30.715
5 ATOM
           320
                N
                     ILE A
                            50
                                     27.009
                                                              1.00 18.34
                                             -1.129
  ATOM
           321
                CA
                    ILE A
                            50
                                     25.874
                                                      31.415
                                                              1.00 19.89
                C
                            50
                                     25.917
                                             -2.629
                                                      31.146
  ATOM
           322
                     ILE A
                                                              1.00 26.29
  ATOM
           323
                0
                     ILE A
                            50
                                     25.322
                                             -3.023
                                                      30.168
                                                              1.00 25.33
  ATOM
           324
                CB
                    ILE A
                            50
                                     24.527
                                             -0.535
                                                      31.008
                                                              1.00 10.50
10 ATOM
           325
                CG1 ILE A
                            50
                                     24.340
                                              0.906
                                                      31.292
                                                              1.00 4.97
  ATOM
           326
                CG2 ILE A
                            50
                                     23.466
                                             -1.298
                                                      31.697
                                                              1.00 12.96
                                     23.413
                                              1.845
                                                      30.602
                                                              1.00 16.65
  MOTA
           327
                CD1 ILE A
                            50
                                     26.707
                                             -3.256
                                                      32.066
                                                              1.00 31.77
                N
                     ARG A
                            51
  ATOM
           328
                CA
                            51
                                     26.887
                                             -4.714
                                                      32.107
                                                              1.00 29.06
  ATOM
           329
                    ARG A
                                             -5.331
                                                      32.170
15 ATOM
           330
                С
                     ARG A
                            51
                                     25.457
                                                              1.00 32.68
   ATOM
           331
                O
                     ARG A
                            51
                                     25.396
                                             -6.363
                                                      31.512
                                                              1.00 37.16
   ATOM
                     ASN A
                            52
                                     24.380
                                             -4.817
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                                                              1.00 28.48
           332
                N
                                             -5.767
                                                      32.832
   ATOM
           333
                CA
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                                     23.284
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   MOTA
           334
                C
                     ASN A
                            52
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20. ATOM
           .335
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                                            -5.884
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                CB
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                                             -6.879
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           338
                OD1 ASN A
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                                             -7.954
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           339
                ND2 ASN A
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25 атом
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                                                              1.00 24.42
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                     ILE A
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                                              -6.151
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           342
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                                              -7.349
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   ATOM
           343
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                     ILE A
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   MOTA
            344
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                     ILE A
                             53
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                                              -4.297
                                                      28.880
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                                              -3.257
30 ATOM
           345
                 CG1 ILE A
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                                     21.682
                                                      27.936
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                                     22.907
                                              -5.321
                                                      27.946
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   ATOM
           346
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                                                      28.383
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40 ATOM
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45 атом
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                     ILE A
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                      ILE A
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50 ATOM
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                     ILE A
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    MOTA
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                                      20.384
                                              -6.460
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                                                               1.00 21.77
            368
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وإليم للمعار والدار ويهييهم الدار ريباني يهارياه بعجاجد

MOTA 369 CD1 ILE A 21.767 -5.582 24.863 1.00 16.23 MOTA 370 N GLN A 56 17.226 -6.412 22.390 1.00 9.67 -7.016 MOTA 371 CA GLN A 56 16.161 21.619 1.00 10.90 16.432 -6.621 20.143 MOTA 372 C GLN A 56 1.00 13.08 5 ATOM 373 0 GLN A 56 16.402 -5.393 19.953 1.00 10.32 14.786 -6.542 22.014 MOTA 374 СB GLN A 56 1.00 11.49 13.653 -7.256 21.316 1.00 23.47 MOTA 375 CG GLN A 56 13.789 -8.741 21.351 1.00 24.88 **ATOM** 376 CD GLN A 56 13.610 -9.379 20.324 1.00 9.56 MOTA 377 OE1 GLN A 56 14.119 -9.221 22.544 1.00 17.94 10 ATOM 378 NE2 GLN A 56 16.288 -7.645 19.216 1.00 6.84 379 GLY A 57 MOTA N GLY A 57 16.174 -7.019 17.841 1.00 16.15 MOTA 380 CA GLY A 57 14.740 -7.085 17.267 1.00 13.72 MOTA 381 C **ATOM** 382 0 GLY A 57 14.124 -8.016 17.752 1.00 12.70 N VAL A 58 14.068 -6.264 16.525 1.00 12.73 15 ATOM 383 12.739 -6.308 16.070 1.00 11.16 **ATOM** 384 CA VAL A 58 12.715 -7.246 14.893 1.00 14.85 MOTA 385 С VAL A 58 VAL A 58 13.234 -6.891 13.849 1.00 18.64 **ATOM** 386 0 12.262 -4.984 15.352 1.00 6.54 **ATOM** 387 CB VAL A 58 **20** ATOM 10.894 -4.974 14.731 1.00 5.89 388 CG1 VAL A 58 CG2 VAL A 58 12.650 -3.840 16.331 1.00 5.86 MOTA 389 MOTA 390 N GLY A 59 12.209 -8.465 15.008 1.00 21.96 CA GLY A 59 MOTA 391 12.120 -9.385 13.874 1.00 17.81 GLY A 59 10.645 -9.561 13.550 1.00 23.35 **ATOM** 392 С GLY A 59 **25** атом 393 9.919 -8.579 13.249 1.00 27.99 0 **ATOM** 394 N GLY A 60 10.166 -10.805 13.623 1.00 18.75 MOTA 8.841 -11.142 13.285 1.00 11.46 395 CA GLY A 60 MOTA 396 С GLY A 8.550 -10.833 11.851 1.00 14.56 60 11.003 MOTA 397 0 GLY A 60 9.160 -11.439 1.00 16.32 7.505 -10.103 **30** ATOM 398 N PRO A 61 11.612 1.00 12.10 399 PRO A 7.123 -9.774 10.250 1.00 14.70 ATOM CA 61 8.230 : -8.941 9.570 1.00 22.17 C PRO A 61 ATOM 400 401 0 8.143 -8.758 8.344 1.00 25.74 ATOM PRO A 61 **ATOM** 402 CB PRO A 61 5.911 -8.860 10.332 1.00 14.30 35 ATOM 5.880 -8.514 11.784 1.00 13.62 403 CG PRO A 61 404 CD PRO A 61 6.723 -9.417 12.576 1.00 12.29 ATOM **ATOM** 405 N TYR A 62 9.162 -8.257 10.292 1.00 21.56 9.973 -7.242 9.674 1.00 17.07 MOTA 406 CA TYR A 62 1.00 18.73 С 11.133 -7.907 9.047 ATOM 407 TYR A 62 -8.213 **40** ATOM 12.132 9.691 1.00 22.39 408 0 TYR A 62 -6.401 MOTA 409 CB TYR A 62 10.504 10.803 1.00 17.51 -5.421 410 CG TYR A 62 11.461 10.236 1.00 15.23 **ATOM** ATOM 411 CD1 TYR A 62 11.343 -4.920 9.032 1.00 17.79 -4.971 10.969 1.00 19.09 MOTA 412 CD2 TYR A 62 12.465 45 ATOM 413 CE1 TYR A 62 12.206 -3.997 8.506 1.00 19.28 MOTA 414 CE2 TYR A 62 13.438 -4.101 10.490 1.00 25.40 MOTA 415 CZ TYR A 62 13.327 -3.571 9.186 1.00 20.95 14.320 -2.649 8.791 1.00 14.70 MOTA 416 OH TYR A 62 7.816 1.00 19.47 MOTA N 63 10.998 -8.419 417 ASP A 50 ATOM 418 CA ASP A 63 12.137 -9.011 7.081 1.00 17.52 1.00 17.97 -7.973 6.453 ATOM 419 С ASP A 63 13.027 -8.442 5.512 1.00 14.94 ATOM 420 0 ASP A 63 13.628 -9.873 6.015 1.00 17.16 MOTA ASP A 63 11.474 421 CB

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               OD2 ASP A 63
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   ATOM
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                CA
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 5 ATOM
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                CB
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10 ATOM
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15 ATOM
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                CB ASN A 69
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                ND2 ASN A 69
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          462
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ATOM
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                N
                                                -0.631 1.00 21.80
 ATOM
          463
                                  8.552
                                          2.619
                    PHE A 70
                CA
          464
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  ATOM
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                    PHE A 70
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                                                -0.724 1.00 25.74
  ATOM
                    PHE A 70
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  ATOM
                   PHE A 70
                CB
 ATOM
          467
                CG PHE A 70
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          468
                CD1 PHE A 70
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  ATOM
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                                           2.314 -4.016 1.00 9.57
 TOM
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   TOM
TOM
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          473
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                                   6.765
                                           2.246
                N
          474
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MOTA 475 CA LEU A 71 5.506 2.725 1.599 1.00 24.24 ATOM 476 С LEU A 71 5.649 4.037 2.343 1.00 27.91 71 6.694 4.521 2.750 477 0 LEU A 1.00 28.86 MOTA 1.635 2.535 478 CB LEU A 71 5.150 1.00 19.99 MOTA 1.873 5.003 0.342 1.00 16.09 5 ATOM 479 CG LEU A 71 -0.764 2.885 1.00 18.12 4.879 480 CD1 LEU A 71 ATOM 3.786 0.546 1.000 1.00 18.24 CD2 LEU A 71 481 ATOM 1.00 33.01 4.535 4.663 2.529 482 N PRO A 72 **ATOM** 4.389 5.888 3.311 1.00 34.96 CA PRO A 72 MOTA 483 5.590 4.778 1.00 32.90 C PRO A 72 4.865 **10 ATOM** 484 4.512 5.331 1.00 28.55 0 PRO A 72 4.619 ATOM 485 3.095 1.00 32.98 486 CB PRO A 72 2.983 6.453 ATOM 2.827 1.00 30.36 2.224 5,189 MOTA 487 CG PRO A 72 2.380 1.00 33.56 3.188 4.093 488 CD PRO A 72 MOTA 5.221 1.00 27.54 73 5.601 6.610 489 N ARG A **15 ATOM** 6.408 1.00 25.42 ARG A 73 6.325 6.547 MOTA 490 CA 6.321 1.00 21.78 5.755 MOTA 491 C ARG A 73 7.613 7.304 1.00 29.61 8.360 5.950 492 0 ARG A 73 MOTA 7.549 1.00 24.29 5.469 5.978 ATOM 493 CB ARG A 73 8.155 1.00 23.47 4.575 6.998 ARG A 73 **20** ATOM 494 CG 6.793 9.360 1.00 29.73 3.818 ARG A 73 MOTA 495 CD 5.460 9.392 1.00 36.30 ARG A 73 3.222 MOTA 496 NE 2.891 5.312 10.713 1.00 42.26 ARG A 73 497 CZ MOTA 11.555 1.00 26.57 NH1 ARG A 73 3.145 6.288 MOTA 498 10.883 1.00 39.03 NH2 ARG A 73 2.320 4.144 25 ATOM 499 5.326 1.00 8.42 4.909 500 GLY A 74 7.868 ATOM N 9.120 4.291 5.332 1.00 5.06 74 MOTA 501 CA GLY A 5.508 1.00 12.74 9.243 2.858 502 C GLY A 74 **ATOM** 5.317 1.00 16.46 10.256 2.286 GLY A 74 MOTA 503 O 2.321 5.906 1.00 12.82 THR A 75 8.145 30 ATOM 504 N 1.00 11.14 505 CA THR A 75 8.036 0.869 6.008 MOTA 75 6.625 0.428 6.134 1.00 10.64 ATOM 506 С THR A 5.949 1.00 9.36 THR A 5.757 1.231 ATOM 507 0 75 7.219 1.00 6.97 8.843 0.398 **ATOM** 508 CB THR A 75 1.00 5.64 8.938 -0.950 7.125 **35** ATOM 75 509 OG1 THR A 8.603 1.00 6.30 8.108 0.865 CG2 THR A 75 ATOM 510 6.409 -0.858 6.259 1.00 10.07 76 **ATOM** SER A 511 N 1.00 13.33 SER A 76 5.061 -1.384 6.354 **ATOM** 512 CA 7.747 1.00 21.87 4.405 -1.163 ATOM 513 C SER A 76 1.00 24.22 5.228 8.679 40 ATOM -1.102 514 0 SER A 76 5.030 -2.832 6.083 1.00 4.81 SER A 76 MOTA 515 CB 7.107 1.00 16.98 76 5.327 -3.664 516 OG SER A MOTA -1.100 3.082 7.911 1.00 24.90 **ATOM** 517 N GLN A 77 1.00 23.85 2.454 -1.020 9.166 GLN A 77 MOTA 518 CA 45 ATOM 2.643 -2.236 10.015 1.00 19.58 GLN A 77 519 С GLN A 77 2.908 -2.140 11.203 1.00 15.15 MOTA 520 0 1.00 32.64 GLN A 77 0.983 -0.703 9.217 MOTA 521 CB 1.00 49.56 0.567 -0.580 10.642 MOTA 522 ÇG GLN A 77 1.00 65.91 0.689 0.785 11.194 GLN A 77 **ATOM** 523 CD 1.00 66.06 50 ATOM 0.956 0.869 12.356 OE1 GLN A 77 524 1.00 68.91 10.350 ATOM NE2 GLN A 77 0.481 1.750 525 9.402 1.00 15.90 -3.376 78 2.754 MOTA 526 N ALA A 1.00 19.47 -4.577 10.073 78 3.071 MOTA 527 ÇA ALA A

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		MOTA	530	CB	ALA		78	3.390	-5.808	9.336	1.00	
		ATOM	531	N	ASN		79	5.350	-3.863	10.093	1.00	
	5	ATOM	532	CA	ASN		79	6.602	-3.576	10.774	1.00	
	•	ATOM	533	C	ASN		79	6.480	-2.673	11.969	1.00	
		ATOM	534	0	ASN		79	6.975	-2.944	13.053	1.00	
		ATOM	535	СВ	ASN		79	7.474	-3.069	9.670	1.00	
		ATOM	536	CG	ASN		79	7.933	-4.238	8.824	1.00	
	10	ATOM	537		ASN		79	7.867	-5.439	9.091	1.00	
		ATOM	538		ASN		79	8.488	-3.891	7.660	1.00	
		ATOM	539	N	ILE		80	5.731	-1.611	11.936	1.00	
		ATOM	540	CA	ILE		80	5.586	-0.574	12.924	1.00	
		ATOM	541	C	ILE		80	4.925	-1.187	14.118	1.00	
	15	ATOM	542	0	ILE		80	5.234	-0.939	15.264	1.00	
	IJ			CB	ILE		80	4.756	0.629	12.436		11.98
		ATOM	543								1.00	
		ATOM	544		ILE		80	5.627	1.124	11.297		9.50
		ATOM	545		ILE		80	4.379	1.728	13.354	1.00	
	20-	ATOM	546		ILE		80	5.007	2.071	10.424	1.00	8.15
	20	ATOM	547	N -	ASP		81	4.017	-2.019	13.708		19.21
		ATOM	548	CA	ASP		81	3.304	-2.778	14.728	1.00	15.15 15.77
		ATOM	549	C	ASP		81	4.147	-3.711	15.510		
		ATOM	550	O	ASP		81	4.084	-3.697	16.695 13.868		15.82
	25	ATOM	551	CB	ASP ASP		81	2.291	-3.438			26.36 23.71
	ZJ	ATOM	552		ASP		81	1.065	-2.530	13.790		23.71 14.33
		MOTA	553	OD1			81	1.105	-1.355	14.226		
		ATOM	554				81	0.061	-3.125	13.222		33.05 16.07
		MOTA	555	N	GLU		82	5.148	-4.447	15.096		14.77
	30	ATOM	556	CA C	GLU		82	5.984	-5.318	15.882		19.33
	30	MOTA	557				82	6.839	-4.355	16.667 17.752		23.58
		MOTA	558	O CB	GLU		82 82	7.315 6.998	-4.708 -6.031	15.064		13.20
ı		ATOM ATOM	559	CG	GLU		82 82	7.792	-7.239	15.476		23.09
ł		ATOM	560 561	CD	GLU		82	6.767	-8.114	16.185		29.68
ı	35		562		GLU		82	5.666	-7.670	16.403		26.63
ı	•••	ATOM	563		GLU		82	7.273	-9.181	16.411		33.08
ı		ATOM	564	N	GLY		83	7.228	-3.227	16.199		16.79
ı		ATOM	565	CA	GLY		83	8.033	-2.428	17.140		17.32
۱		MOTA	566	C	GLY		83	7.238	-2.018	18.366		17.54
١	40		567	o	GLY		83	7.561	-2.103	19.528		15.06
١		ATOM	568	N	LYS		84	6.093	-1.408	18.114		18.72
١		ATOM	569	CA	LYS		84	5.050	-1.146	19.096		16.90
1		ATOM	570	C	LYS		84	4.893	-2.337	20.057		17.74
١		ATOM	571	ō	LYS		84	4.962	-2.265	21.295		14.31
1	45	ATOM	572	CB	LYS		84	3.799	-0.872	18.307		14.62
١		ATOM	573	CG	LYS		84	3.535	0.565	18.291		19.30
١		ATOM	574	CD	LYS		84	2.787	1.013	17.044		34.24
1		ATOM	575	CE	LYS		84	1.568	1.902	17.337		37.70
		ATOM	576	NZ	LYS		84	0.346	1.226	16.827		48.42
State of the same of	50		577	NZ N	ARG		85	4.617	-3.506	19.519		18.50
1	"	ATOM	578	CA	ARG		85	4.517	-4.705	20.280		19.04
17.		ATOM	579	CA	ARG		85	5.677	-4.733	21.308		19.63
		ATOM	580	0	ARG		85	5.442	-5.192	22.383		19.24
rielan		ALON	500	9	ARG		33	J. 774	2.172	20.303	2.00	~~

		ATOM	581	СВ	ARG A	85		4.740	-5.979	19.464	1.00	14.74
		ATOM	582	CG	ARG A	85		3.843	-7.094	19.887	1.00	8.85
		ATOM	583		ARG A	85		4.146	-8.554	19.705	1.00	7.20
		ATOM	584		ARG A	85		5.483	-8.898	19.194	1.00	
	5	ATOM	585		ARG A	85		6.170	-9.705	19.899		18.19
	Ŭ	ATOM	586		ARG A	85			-10.161	21.040		34.03
		ATOM	587		ARG A	85		7.345	-9.979	19.555		15.36
		ATOM	588		LEU A	86	•	6.901	-4.586	20.956		22.21
				CA	LEU A	86		8.006	-4.792	21.873		20.94
	40	MOTA	589		LEU A	86		8.044	-3.637	22.803		20.73
	IU	MOTA	590						-3.970	23.925		22.18
		MOTA	591		LEU A	86		8.155	-4.932	21.168	1.00	6.67
		ATOM	592	CB	LEU A	86		9.333		20.282		11.45
		MOTA	593	CG	LEU A	86		9.358	-6.241			
	4-	MOTA	594		LEU A	86		10.546	-6.054	19.287		18.60
	15	MOTA	595		LEU A	86		9.362	-7.516	21.020	1.00	5.17
		MOTA	596	N	PHE A	87		7.700	-2.446	22.529		16.79
		MOTA	597	CA	PHE A	87		7.850	-1.416	23.492		18.21
		MOTA	598	C	PHE A	87		6.939	-1.805	24.618		26.51
		MOTA	599	0	PHE A	87		7.082	-1.565	25.839		30.36
	20	ATOM	600	CB	PHE A	87			-0.118	22.846		15.81
		MOTA	601	CG	PHE A	87		8.661	0.503	22.128		22.72
		MOTA	602	CD1	PHE A	87		9.625	1.163	22.795		25.90
		MOTA	603	CD2	PHE A	87		8.800	0.446	20.774		24.19
l		ATOM	604	CE1	PHE A	87		10.699	1.781	22.220	-	26.46
ı	25	MOTA	605	CE2	PHE A	87		9.871	0.991	20.153		29.24
١		MOTA	606	CZ	PHE A	87		10.827	1.669	20.849		20.81
l		ATOM	607	N	ALA A	88		5.862	-2.422	24.266		29.15
١		MOTA	608	CA	ALA A	88		4.772	-2.699	25.195		22.92
١		MOTA	609	C	ALA A	88		5.186	-3.837	26.06B		22.03
١	30	ATOM	610	0	ALA A	88		4.974	-3.879	27.284	1.00	27.02
١		MOTA	611	СВ	ALA A	88		3.551	-2.803	24.299	1.00	22.13
١		MOTA	612	N	LEU A	89		5.649	-4.897	25.531		19.16
١		MOTA	613	CA	LEU A	89		6.188	-6.032	26.208	1.00	19.29
١		MOTA	614	С	LEU A	89		7.250	-5.507	27.133	1.00	22.06
١	35	MOTA	615	0	LEU A	89		7.449	-6.050	28.177	1.00	20.49
1		MOTA	616	CB	LEU A	89		7.021	-6.863	25.221	1.00	18.41
١		ATOM	617	CG	LEU A	89		7.477	-8.167	25.834	1.00	20.45
1		MOTA	618	CD1	LEU A	89		6.326	-8.707	26.627	1.00	17.22
1		MOTA	619	CD2	LEU A	89		8.060	-9.057	24.769	1.00	18.83
	40	MOTA	620	N	ALA A	90		8.124	-4.644	26.722		22.80
		MOTA	621	CA	ALA A	90		9.027	-4.137	27.701	1.00	24.14
		MOTA	622	C	ALA A	90		8.237	-3.488	28.849		23.63
		ATOM	623	0	ALA A	90		8.414	-3.835	30.071	1.00	22.73
		ATOM	624	CB	ALA A	90		10.080	-3.253	27.139	1.00	7.74
	45	MOTA	625	N	ASN A	91		7.457	-2.445	28.732	1.00	25.45
	1	MOTA	626	CA	ASN A			6.665	-1.979	29.870	1.00	27.25
	1	ATOM	627	С	ASN A			5.847	-2.996	30.656	1.00	30.97
	1	ATOM	628	ō	ASN A			5.346			1.00	27.64
	1:		629		ASN A			5.560				29.14
·	Š	MOTA	630		ASN A			4.946				31.73
	1	ATOM	631		ASN A			3.845				46.76
	1	ATOM	632		2 ASN A			5.641				29.03
	3	ATOM	633		GLN A			5.369				35.37
	1	ATOP1	0.5.5	14	92K A							

4.702 -5.141 30.591 1.00 35.55 **ATOM** 634 CA GLN A 92 -6.072 5.619 31.352 1.00 34.28 ATOM 635 C GLN A 92 GLN A 5.227 -6.519 32.440 1.00 39.47 MOTA 636 92 ATOM 637 GLN A 92 3.866 -5.903 29.573 1.00 54.94 2.689 -6.698 30.142 1.00 78.63 ATOM 638 GLN A 92 2.806 -8.167 29.805 1.00 93.87 MOTA 639 GLN A 92 3.597 -8.840 30.475 1.00 96.99 MOTA 640 OE1 GLN A 92 **ATOM** 641 NE2 GLN A 92 2.083 -8.696 28.824 1.00 97.81 ATOM 642 N LYS A 93 6.859 -6.403 31.050 1.00 31.97 -7.204 **10** ATOM 643 CA LYS A 93 7.675 31.972 1.00 25.22 -6.298 33.015 1.00 24.68 **ATOM** 644 С LYS A 93 8.381 -6.793 34.075 1.00 32.13 MOTA 645 0 LYS A 93 8.716 -7.980 31.148 1.00 10.86 MOTA 646 CB LYS A 93 B.673 -8.963 30.159 1.00 24.26 ATOM 647 CG LYS A 93 8.225 -9.966 29.986 1.00 21.96 LYS A 9.362 **15** ATOM 648 CD 93 9.093 -10.718 28.658 1.00 23.78 LYS A ATOM 649 CE 93 10.084 -11.805 28.300 5.00 25.87 LYS A **ATOM** 650 NZ 93 ATOM 651 N CYS A 94 8.752 -5.096 32.774 1.00 16.62 9.752 -4.412 33.480 1.00 18.95 **ATOM** 652 CA CYS A 94 -2.936 33.537 1.00 24.83 20 ATOM С CYS A 9.512 653 94 10.184 -2.017 33.150 1.00 26.80 **ATOM** 0 CYS A 94 654 **ATOM** 655 CYS A 94 11.147 -4.691 32.911 1.00 3.14 CB -6.437 32.882 1.00 25.28 ATOM 656 SG CYS A 94 11.618 8.403 -2.561 34.086 1.00 26.08 **ATOM** 657 N PRO A 95 25 атом CA PRO A 7.891 -1.202 33.878 1.00 26.11 658 95 ATOM 659 C PRO A 95 B.960 -0.259 34.299 1.00 27.32 MOTA 660 0 PRO A 95 8.776 0.966 34.108 1.00 29.08 1.00 20.75 -1.090 34.747 661 CB 6.609 MOTA PRO A 95 6.587 -2.421 35.322 1.00 19.04 MOTA 662 CG PRO A 95 -3.461 30 ATOM 663 CD PRO A 95 7.363 34.509 1.00 22.55 664 ASN A 9.836 -0.776 35.193 1.00 31.44 **ATOM** N 96 MOTA 665 CA ASN A 96 10.559 0.274 35.966 1.00 35.38 0.476 35.353 MOTA 666 С ASN A 96 11.891 1.00 33.83 **ATOM** 667 0 ASN A 96 12.599 1.359 35.684 1.00 33.31 35 ATOM 668 CB ASN A 96 10.558 -0.099 37.429 1.00 53.70 MOTA 669 CG ASN A 96 9.238 0.342 38.026 1.00 61.69 37.706 8.758 1.432 1.00 64.33 MOTA 670 OD1 ASN A 96 38.861 1.00 67.25 MOTA 671 ND2 ASN A 8.676 -0.526 96 -0.409 34.507 1.00 30.32 ATOM 672 12.287 N THR A 97 40 ATOM THR A -0.367 33.794 1.00 22.83 673 CA 97 13.519 MOTA 674 C THR A 97 13.404 0.493 32.534 1.00 22.44 MOTA 675 0 THR A 97 12.446 0.779 31.816 1.00 21.14 MOTA 676 -1.851 33.705 1.00 25.87 CB THR A 97 13.835 MOTA 677 14.602 -1.915 32.528 1.00 38.91 OG1 THR A 97 45 ATOM 678 CG2 THR A 97 12.769 -2.901 33.621 1.00 24.22 MOTA 679 PRO A 14.393 1.415 32.408 1.00 20.59 N 98 31.254 1.00 18.15 MOTA ' 680 CA PRO A 98 14.513 2.292 1.00 16.07 ATOM C PRO A 98 14.882 1.494 29.978 681 MOTA 0.462 29.934 1.00 17.19 682 0 PRO A 98 15.622 ATOM 3.339 31.676 1.00 14.55 683 CB PRO A 98 15.563 ATOM 684 CG PRO A 98 16.270 2.646 32.699 1.00 12.29 MOTA CD 33.046 1.00 12.02 685 PRO A 98 15.735 1.331 ATOM 686 28.940 1.00 13.81 VAL A 14.322 2.107 N 99

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MOTA 687 CA VAL A 14.225 1.544 27.632 1.00 14.02 MOTA 688 C VAL A 14.956 2.407 1.00 10.66 99 26.663 MOTA 689 0 VAL A 99 14.716 3.679 26.712 1.00 6.90 **MOTA** 690 CB VAL A 99 12.673 1.343 27.335 1.00 2.87 5 ATOM 691 CG1 VAL A 99 12.666 1.272 25.872 1.00 17.40 MOTA 692 CG2 VAL A 99 12.442 -0.111 27.744 1.00 5.75 , MOTA 693 N **VAL A 100** 15.885 1.776 25.861 1.00 6.45 MOTA 694 CA VAL A 100 16.525 2.755 24.900 1.00 9.61 MOTA 695 С **VAL A 100** 16.389 2.159 23.561 1.00 10.79 10 ATOM 696 0 VAL A 100 16.256 0.973 23.477 1.00 MOTA 697 CB VAL A 100 17.877 3.260 25.197 1.00 8.05 CG1 VAL A 100 MOTA 698 17.824 4.252 26.336 1.00 6.05 MOTA 699 CG2 VAL A 100 2.053 25.591 18.853 1.00 6.68 **ATOM** 700 N **ALA A 101** 2.928 16.277 22.511 1.00 13.14 **15** ATOM 701 ALA A 101 2.266 21.183 CA 16.127 1.00 15.67 **ATOM** 702 C ALA A 101 17.065 2.747 20.053 1.00 12.08 **ATOM** 703 Ω ALA A 101 17.261 4.042 19.907 1.00 11.16 **ATOM** 704 CB ALA A 101 14.685 2.609 20.812 1.00 6.57 ATOM 705 **GLY A 102** 17.218 1.00 N 1.787 19.099 7.53 20 ATOM 706 CA **GLY A 102** 17.949 2.415 17.939 1.00 7.10 ATOM 707 С **GLY A 102** 17.477 1.803 16.744 1.00 7.27 MOTA 708 0 GLY A 102 17.102 0.621 16.878 1.00 10.83 **MOTA** 709 N **GLY A 103** 17.706 2.407 15.648 1.00 7.80 MOTA 710 CA **GLY A 103** 17.446 1.745 14.356 1.00 5.33 25 атом 711 C 18.303 **GLY A 103** 2.211 13.180 1.00 MOTA 712 0 **GLY A 103** 18.785 3.340 13.227 1.00 MOTA 713 N **TYR A 104** 18.490 1.387 12.139 1.00 7.09 MOTA 714 CA TYR A 104 19.392 1.682 11.069 1.00 5.99 715 C TYR A 104 18.705 1.00 **MOTA** 1.614 9.705 9.47 30 ATOM TYR A 104 716 0 18.115 0.638 9.441 1.00 6.46 ATOM 11.079 1.00 717 CB TYR A 104 20.592 0.797 5.40 MOTA 718 CG **TYR A 104** 21.436 1.078 9.876 1.00 8.05 **ATOM** 719 CD1 TYR A 104 21.708 2.302 9.352 1.00 5.91 **MOTA** 720 CD2 TYR A 104 21.961 -0.044 9.172 1.00 6.85 35 ATOM 721 CE1 TYR A 104 22.447 2.513 8.186 1.00 5.61 MOTA 722 CE2 TYR A 104 22.751 0.052 8.072 1.00 7.49 MOTA 723 CZ**TYR A 104** 22.972 1.377 7.608 1.00 11.08 MOTA 724 OH **TYR A 104** 23.795 1.509 6.479 1.00 14.32 MOTA 725 N **SER A 105** 18.939 2.975 8.852 1.00 18.39 **40** ATOM 726 CA SER A 105 18.190 2.854 7.601 1.00 9.66 MOTA 727 16.763 C **SER A 105** 2.370 7.722 1.00 6.10 **ATOM** 728 0 **SER A 105** 16.090 3.304 8.077 1.00 5.63 **ATOM** 729 CB **SER A 105** 19.124 2.159 6.607 1.00 8.55 **ATOM** 730 OG **SER A 105** 18.553 5.463 1.685 1.00 24.30 45 ATOM 731 N **GLN A 106** 16.241 1.405 7.079 1.00 9.93 MOTA 14.759 7.002 732 CA **GLN A 106** 1.316 1.00 8.25 **ATOM GLN A 106** 14.453 8.473 733 C 1.089 1.00 8.51 1.00 MOTA 734 **GLN A 106** 13.470 8.862 0 1.6B3 6.31 ATOM 735 CB **GLN A 106** 14.239 0.393 5.940 1.00 7.45 50 ATOM 1.00 18.04 736 CG **GLN A 106** 13.184 -0.528 6.465 **ATOM** 737 CD **GLN A 106** 12.228 -1.220 5.581 1.00 16.87 **ATOM** 738 OE1 GLN A 106 11.024 -1.180 5.492 1.00 17.59 ATOM 739 NE2 GLN A 106 12.643 -2.032 4.713 1.00 8.32

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1.00 7.13 9.172 15 o.310 4.61 1.00 10.606 0.159 269 1.00 8.27 11.356 1.472 190 048 6.52 15 1.00 12.290 1.511 15 1.00 11.033 2.637 15 7.41 219 653 1.00 11.641 3.864 14 1.00 11.76 11.471 4.346 1 12.64 1.00 266 813 01 12.298 4.914 15 1.00 13.93 11.170 13. 5.006 13 · 813 13 · 150 13 · 121 16 · 321 13 · 056 12 · 096 11 · 016 10 · 035 9.78 1.00 10.267 4.312 $G^{L^{Y}}$ 1.00 10.47 9.861 4.685 1.00 12.32 10.727 3.858 1.00 14.67 11.035 140 4.391 1.00 10.24 142 143 144 145 146 147 148 148 149 150 8.456 4.173 4.34 1.00 11.077 2.690 10.035 12.259 11.458 10.305 10.298 1.00 11.71 11.783 1.760 1.00 15.26 13.203 2.253 1.00 18.07 2.672 13.685 7.52 1.00 11.634 9.298 0.319 1.00 8.41 12.258 -0.801 9 · 231 11 · 247 10 · 685 10 · 278 10 · 397 11 · 510 11 · 027 1.00 7.17 11.862 -2.233 A TON A TON 1.00 5.25 13.783 -0.659 1.00 15.77 13.907 2.373 1.00 12.22 ATOM ATOM ATOM ATOM ATOM ATOM ATOM 15.246 2.860 9.39 1.00 15.234 4.255 1.00 12.54 16.241 11.0274.636 1.00 15.55 15.685 10.404 2.814 1.00 14.19 15.805 12.917 1.279 4.64 1.00 17.005 12 . 97 12 . 225 13 . 190 12 . 309 11 . 792 10 . 266 8 . 334 3.465 1.00 14.88 17.002 0.887 1.00 11.00 14.341 5.170 1.00 12.45 14.427 6.528 1.00 15.59 14.30B 6·455 1.00 18.13 15.154 7.1315.70 1.00 13.486 7.505 1.00 12.85 13.587 11.334 5.572 1.00 15.39 13.557 ATOM B.575 5.512 1.00 18.21 14.861 ATOM 5.093 167 1.00 14.59 ATOM ATOM 15.226 5.750 1.6.6 415 1.00 17.63 12.500 4.562 498 1.00 16.02 ATOM 15.303 3.948 1.00 16.43 618 ATOM 16.412 3.218 937 1.00 22.20 ATOM 17.643 4.114 483 1.00 18.94 ATOM 18.426 4.321 6 518 ATOM 4.69 1.00 16.565 2.084 114 114 114 114 115 115 115 613 ATOM 6 1.00 22.46 17.744 4.836 5 474 1.00 20.88 ATOM 19.064 ATOM 1. 122 5.499 22.71 1.00 19.007 6.469 7.855 1. 1.00 22.05 20.057 6.761 6.670 1.00 19.61 19.137 6.090 6.136 1.00 8.35 20.122 9.279 1.00 13.91 7.259 19.562 5.016 .396 1.00 23.59 115 17.828 9 245 7.085 10. 6.467 115 115 ,G2

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					16			
			SER A	116	5.539	8.172	17.736	1.00 23.68
	193	CA	SER A		4.169	7.647	18.120	1.00 23.77
	194	C O	SER A	116	3.333	8.523	18.399	1.00 27.35
	197	CB	SER A		5.522	8.865	16.376	1.00 25.21
<i>A</i>	.06	0G	SER A		5.168	8.043	15.277	1.00 28.05
S	19'	N	GLU A		3.859	6.397	18.004	1.00 18.83
NEN.	190	СA	GLU A		2.491	6.020	18.238	1.00 22.21
2015	497	C	GLU A		2.461	5.474	19.653	1.00 30.46
a 6.05 S	200	0	GLU A		1.487 1.977	4.773 4.902	19.863 17.343	1.00 35.72
To BOUT S	~0-	CB	GLU A		2.167	5.219	15.897	1.00 21.63
San Contract	~0~	CG	GLU A		1.560	4.424	14.814	1.00 34.01
1000	-0-	CD	GLU A		0.912	3.440	15.046	1.00 32.59
1000	B 0 4	0E1	GLU A		1.750	4.833	13.659	1.00 44.62
10 8 5 0 EN	-0-	OE2	LEU A		3.438	5.570	20.512	1.00 34.45
SA COSO	B06	N	LEU A	118	3.326	5.006	21.812	1.00 33.64
- 6606	B07 B08	CA	LEU A	118	2.681	6.110	22.633	1.00 41.75
P5051	809	C	LEU A		2.594	7.267	22.370	1.00 39.90
0 8600	-1"	O CB	LEU A		4.600	4.668	22.392	1.00 29.44
1 7500	- 1	CG	LEU A		5.628	3.891	21.645	1.00 26.36
7 3 O'A	41-	CD^{1}	LEU A		6.921	3.840	22.379	1.00 27.53
1000	- 1	CD2	LEU A		5.110 2.076	2.520	21.536 23.726	1.00 20.69
1 10 Prost	- 1 -	N	SER A		0.910	5.794 5.647	23.726	1.00 48.86 1.00 52.44
P3 Ora		CA	SER A		1.212	6.063	25.866	1.00 52.44
1 2 OF		C	SER A		1.485.	5.258	26.735	1.00 55.54
1 200		0	SER A		0.550	4.132	24.488	1.00 70.55
20 23.01		CB	SER A		1.393	3.091	23.908	1.00 66.80
PIOT	-1/	OG.	GLY A	120	1.532	7.307	26.024	1.00 52.95
Pron	- A'A	N	GLY A		1.910	7.761	27.382	1.00 53.35
PAOL	821	CA C	GLY A		2.944	7.109	28.291	1.00 49.09
To Proper	822 823 824	0	GLY A		4.086	7.617	28.358	1.00 49.66
A PON	474	Ŋ	ALA A		2.526 3.477	6.129 5.574	29.102 30.022	1.00 42.97
A TOM	.7.2	CA	ALA A		4.587	4.772	29.326	1.00 44.20
P 01	, .	C	ALA A		5.749	4.803	29.711	1.00 45.42
P OF		0	ALA A		2.965	4.542	30.903	1.00 36.34
Pro	4.2	CB	VAL A	122	4.122	4.035	28.312	1.00 41.15
10,	. 12.7	N	VAL A		5.090	3.269	27.548	1.00 33.41
N. C.	49	CA	VAL A		5.870	4.168	26.652	1.00 28.48
L'ON	β31 β32	С 0	VAL A		7.084	4.019	26.872	1.00 27.69
2,01		CB	VAL A		4.424	2.056	26.952	1.00 30.22
rou		CG1	VAL A	122	2.924 4.891	1.997 1.836	27.098 25.551	1.00 28.03 1.00 23.22
road		CG^2	LYS A	123	5.424	5.310	26.177	1.00 23.22
70	836 831	N	LYS A	123	6.354	6.314	25.661	1.00 23.11
TOM		CA	LYS A	123	7.403	6.783	26.661	1.00 25.28
TO A	838	С	LYS A	123	8.524	7.224	26.449	1.00 29.01
		0	LYS A	123	5.561	7.502	25.100	1.00 23.54
		CB	LYS A	123	6.171	8.573	24.277	1.00 26.71
Or of	- 4 -	CG	LYS A	123	5.400	9.775	23.888	1.00 43.07
100	- 4 -	CD	T.YS A	123	4.953	9.783	22.461	1.00 59.59
		CB NZ	LYS A	123	3.518	9.637	22.099	1.00 67.50
		ND						
	84							
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	. 19 ⁹⁸							

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                     LEU A 131
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                                                    13.661
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		MOTA		900	CB	LEU	A	131	17.604	7.713	14.102	1.00	8.40
		MOTA		901	CG	LEU	A	131	16.160	7.830	14.575	1.00	6.67
		MOTA		902	CD1	LEU	A	131	15.391	8.957	13.981	1.00	4.49
	5	MOTA		903	CD2	LEU	A	131	15.481	6.488	14.324	1.00	5.12
		MOTA		904	N	PHE	A	132	20.271	6.009	12.802	1.00	11.56
		MOTA		905	CA	PHE	A	132	21,422	6.183	11.908		10.44
		MOTA		906	С	PHE	A	132	20.965	6.013	10.478	1.00	8.46
		MOTA		907	0	PHE	А	132	20.175	5.101	10.097		11.04
	10	MOTA	,	908	CB	PHE	A	132	22.217	4.931	12.282		10.56
		ATOM		909	CG			132	22.693	4.830	13.714		16.38
		ATOM		910		PHE			21.951	4.029	14.542		13.36
		ATOM		911		PHE			23.860	5.489	14.213		15.12
		ATOM		912	CE1				22.342	3.911	15.889		14.91
	15	ATOM		913		PHE			24.176	5.323	15.513		18.02
		ATOM		914	cz			132	23.426	4.530	16.403		15.09
		ATOM		915	N			133	21.431	6.876	9.580	1.00	7.35
		ATOM		916	CA			133	21.026	6.893	8.148	1.00	5.86
		ATOM		917	C			133	19.503	6.919	8.061		12.25
	20	ATOM		918	0.			133					
	20	ATOM		919	N			134	18.890	5.926	7.593	1.00	9.03
		ATOM		920	CA			134	18.926	8.070	8.532	1.00	9.85
		ATOM		921	C			134	17.455	8.022	8.838	1.00	7.40
		ATOM			0				16.647	8.365	7.584		10.61
	25	ATOM		922				134	16.785	9.513	7.131	1.00	5.85
	23			923	CB			134	17.161	9.128	9.836	1.00	7.27
		MOTA		924	CG			134	15.842	9.393	10.391	1.00	7.89
ŀ		ATOM		925	CD1			134	14.889	8.437	10.312	1.00	6.65
		ATOM		926		TYR			15.661	10.651	10.948		11.44
١	30	MOTA MOTA		927		TYR			13.657	8.690	10.821	1.00	9.05
	30			928	CE2			134	14.408	10.928	11.467		12.89
١		ATOM		929	CZ			134	13.428	9.923	11.423		14.22
١		MOTA		930	OH			134	12.146	10.110	11.975		12.41
١		MOTA		931	N			135	15.811	7.398	7.139		11.51
١	35	ATOM ATOM		932	CA			135	15.229	7.581	5.789	1.00	7.71
١	00	ATOM		933	C O			135	14.082	8.530	5.825		10.36
ı		ATOM		934 935	СВ			135	13.845	8.878	4.727		11.26
1		ATOM		936				135 135	14.772	6.394	4.967		12.02
1		ATOM		937				135	13.821	5.399	5.398		22.81
1	40				N CG2			136	15.828	5.332	4.712		14.88
1		ATOM		938 939	CA				13.632	9.105	6.928		15.28
Accession.	٠.	ATOM			CA			136 136	12.596	10.134	6.968		16.48
4				940	0				13.102	11.418	7.646		17.46
31	1	ATOM		941				136	12.292	12.231	8.035		12.82
á	45	ATOM		942	CB			136	11.336	9.671	7.701	1.00	
₹	Y.	ATOM		943	CG			136	11.178	8.191	7.263		13.60
j	1	ATOM		944	CD			136	10.504	8.264	5.932		14.65
4	7	ATOM		945				136	9.587	9.102	5.986		23.99
盤	X	ATOM		946				136	10.852	7.529	4.914		14.68
ě	th	ATOM		947	N			137	14.421	11.532	7.566		18.52
1	E.	MOTA		948	CA			137	14.953	12.752	8.141		18.16
The state of the s	1	ATOM		949	C			137	14.301	13.929	7.458		19.79
3	1	ATOM		950	0			137	13.895	14.802	8.157		12.28
The Assessment	The same of the sa	ATOM		951	CB	ASN	A	137	16.481	12.573	8.239	1.00	14.17

		ATOM	952	CG	ASN	Α	137	17.247	13.740	8.812	1.00	19.75
		MOTA	953	OD1	ASN	A	137	17.821	14.341	7.934	1.00	14.52
		MOTA	954	ND2	ASN	A	137	17.390	14.130	10.042		17.43
		ATOM	955	N	LEU	Α	138	14.180	14.062	6.141	1.00	27.31
	5	MOTA	956	CA	LEU	A	138	13.640	15.270	5.553	1.00	
		ATOM	957	C	LEU	Α	138	12.190	15.332	5.971	1.00	
		MOTA	958	0	LEU	A	138	11.710	16.281	6.549		25.13
		ATOM	959	CB	LEU	Α	138	13.632	15.269	4.056		41.28
		ATOM	960	CG	LEU			13.713	16.582	3.303		31.76
1	0	ATOM	961	CD1	LEU	A	138	14.641	17.503	4.012		51.09
		ATOM	962		LEU			14.207	16.573	1.958		46.20
		ATOM	963	N	GLN			11.378	14.403	5.569		20.48
		ATOM	964	CA	GLN			10.034	14.390	6.037		19.98
		ATOM	965	С	GLN			9.846	14.749	7.471		22.85
1	15	ATOM	966	0	GLN			8.791	15.282	7.528		26.66
		ATOM	967	СВ	GLN			9.517	12.969	5.899		18.37
		ATOM	968	CG	GLN			9.684	12.643	4.450		22.02
		ATOM	969	CD			139	10.984	11.983	4.110		22.69
		ATOM	970		GLN			10.504	10.980	3.477		35.62
	วก	ATOM	971				139	12.195		4.410		3170
	LU	ATOM	972	N			140	10.454	14.072	8.427		26.14
		ATOM	973	CA			140	10.434	14.183	9.848		19.06
l		MOTA	974	C			140	10.213	15.429	10.293		16.99
		ATOM	975	0			140					18.05
	25	ATOM	976	CB			140	11.040	15.654	11.454 10.541		
'	23	ATOM	977	CG			140	10.581	12.910			17.20 16.28
ı					ASN			9.465	11.998 12.565	10.210		23.57
l		ATOM ATOM	978 979		ASN			8.615		9.563		
1				ND2				9.460	10.756	10.630 9.397		22.65
l	30	ATOM ATOM	980	CA			141 141	11.457	16.162			19.20
1	00		981 982	C				12.170	17.350	9.790		26.25
3		ATOM ATOM	983	0			141 141	13.219 13.365	17.090	10.818		25.06
3		ATOM	984	СВ			141	11.123	17.928 18.299	11.649 10.271		27.60 37.72
3		ATOM	985	CG			141		18.974	9.372		49.61
	35	ATOM	986	N			142	10.083 14.110	16.165	10.920		19.42
		ATOM	987	CA			142	14.110	15.778	11.902		14.21
3		ATOM	988	C			142	14.652	15.776	13.158		19.42
The state of the s	:	ATOM	989	0			142	15.547	14.759	13.130		23.74
7	â	ATOM	990	N			143	13.354	14.851	13.569		14.09
	動	MOTA	991	CA			143	13.334	14.075	14.757		11,80
薯	to the second	MOTA	992	C			143	12.203	12.972	14.757		16.69
2	3	ATOM	993	0			143	11.760	12.787	13.481		19.57
		ATOM	994	N			144	11.668	12.787	15.590		19.71
	*	ATOM	995				144					
	\$	ATOM		CA			144	10.494	11.589	15.667		20.13 27.00
7	4		996	C				9.313	12.315	16.296		
4	多	MOTA	997	O			144	9.298	13.026	17.268		26.75
	Ť	ATOM	998	CB			144	10.973	10.583	16.692		16.84
	4	ATOM	999				144	12.363	9.956	16.348	1.00	
1		ATOM	1000				144	9.882	9.636	16.775		14.01
1	25	ATOM	1001				144	12.437	9.156	17.562	1.00	2.75
		MOTA	1002	N			145	8.249	12.380	15.499		32.77
1		ATOM	1003	CA			145	6.959	12.993	15.779		29.89
		ATOM	1004	С	PRC	A	145	6.484	12.588	17.180	1.00	27.78
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MOTA 1005 O PRO A 145 6.475 11.446 17.537 1.00 26.07 1006 PRO A 145 MOTA CB 5.957 12.384 14.784 1.00 26.51 **ATOM** 1007 CG PRO A 145 6.887 12.059 13.668 1.00 25.85 1008 CD PRO A 145 **ATOM** 8.174 11.563 14.234 1.00 31.33 1009 **ASN A 146** MOTA N 5.796 13.462 17.878 1.00 27.07 ATOM 1010 CA **ASN A 146** 5.454 13.274 19.230 1.00 28.59 MOTA 1011 С **ASN A 146** 6.526 12.605 20.045 1.00 29.25 ATOM 1012 0 **ASN A 146** 6.087 11.995 20.996 1.00 35.51 1013 **ATOM** CB **ASN A 146** 4.285 12.364 19.230 1.00 41.13 **10 ATOM** 1014 CG **ASN A 146** 3.300 12.568 18.120 1.00 48.43 ATOM 1015 OD1 ASN A 146 3.134 13.721 17.788 1.00 49.24 ATOM 1016 ND2 ASN A 146 2.763 11.437 17.695 1.00 47.79 ATOM 1017 N **TYR A 147** 7.791 12.799 19.885 1.00 23.88 ATOM 1018 CA **TYR A 147** 8.689 12.339 20.969 1.00 21.90 15 ATOM 1019 С **TYR A 147** 9.583 13.495 21.285 1.00 22.57 MOTA 1020 0 **TYR A 147** 9.777 14.399 20.494 1.00 26.53 **ATOM** 1021 CB **TYR A 147** 9.309 11.098 20.498 1.00 21.16 MOTA TYR A 147 1022 CG 10.285 10.471 21.349 1.00 20.45 **ATOM** 1023 CD1 TYR A 147 9.882 9.720 22.384 1.00 24.28 20 ATOM 1024 CD2 TYR A 147 11.608 10.564 21.189 1.00 17.96 ATOM 1025 **CE1 TYR A 147** 10.681 9.029 23.273 1.00 24.55 **ATOM** 1026 CE2 TYR A 147 12.509 9,948 21.983 1.00 20.73 ATOM 1027 CZ **TYR A 147** 12.022 23.030 9.184 1.00 24.61 MOTA 1028 OH **TYR A 147** 12.891 8.536 23.887 1.00 24.80 25 ATOM 1029 N PRO A 148 9.893 13.858 22.507 1.00 22.86 **ATOM** 1030 CA PRO A 148 10.817 14.916 22.769 1.00 21.77 ATOM 1031 С PRO A 148 12.127 14.882 21.957 1.00 22.49 **ATOM** 1032 0 PRO A 148 13.007 14.004 22.117 1.00 22.31 ATOM 1033 CB PRO A 148 11.185 14.694 24.251 1.00 23.23 **30 ATOM** 1034 CG PRO A 148 10.324 24.719 13.576 1.00 23.39 ATOM 1035 CD PRO A 148 9.677 12.889 23.590 1.00 25.33 MOTA 1036 N ARG A 149 12.432 15.980 21.250 1.00 25.45 13.735 ATOM 1037 CA ARG A 149 16.138 20.567 1.00 22.54 ATOM 1038 C ARG A 149 14.910 16.018 21.499 1.00 21.28 35 ATOM 1039 0 ARG A 149 15.860 15.477 21.015 1.00 16.61 **ATOM** 1040 CB ARG A 149 13.829 17.346 19.727 1.00 31.02 MOTA 1041 CG ARG A 149 12.837 17.750 18.719 1.00 58.26 MOTA 1042 ARG A 149 CD 13.452 18.605 17.658 1.00 80.58 ATOM ARG A 149 1043 NE 13.769 17.798 16.491 1.00 92.05 **40** ATOM 1044 CZARG A 149 13.315 18.154 15.320 1.00 91.85 NH1 ARG A 149 ATOM 1045 1.00 86.98 12.586 19.213 15.165 MOTA 1046 NH2 ARG A 149 13.544 17.488 14.242 1.00 91.61 14.813 MOTA 1047 N **GLU A 150** 16.282 22.825 1.00 28.09 **ATOM** 1048 CA **GLU A 150** 15.950 16.171 23.735 1.00 25.55 45 ATOM 1049 C **GLU A 150** 16.272 14.736 24.020 1.00 21.12 ATOM 1050 0 **GLU A 150** 17.372 14.443 24.371 1.00 24.39 ATOM 1051 CB **GLU A 150** 15.753 17.040 24.917 1.00 38.73 MOTA 1052 CG **GLU A 150** 14.328 17.370 25.359 1.00 67.27 **GLU A 150** 26.899 MOTA 1053 CD 14.252 17.185 1.00 85.05 MOTA 0 1054 OE1 GLU A 150 15.005 17.890 27.657 1.00 90.70 **ATOM** 1055 OE2 GLU A 150 13.454 16.321 27.373 1.00 91.68 **ATOM** 1056 N ARG A 151 15.396 13.807 23.727 1.00 19.70 **ATOM** 1057 CA ARG A 151 15.752 12.424 23.844 1.00 19.52

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MOTA 1111 **ASN A 157** 27.115 10.714 8.300 1.00 30.34 MOTA 1112 CG **ASN A 157** 27.733 9.498 7.932 1.00 34.95 1113 OD1 ASN A 157 8.573 MOTA 28.011 8.606 1.00 44.28 ND2 ASN A 157 27.965 9.541 MOTA 1114 6.660 1.00 54.18 ATOM 1115 N VAL A 158 26.849 13.501 6.313 1.00 25.65 1116 CA **VAL A 158** 26.825 14.483 5.192 MOTA 1.00 28.21 VAL A 158 26.768 13.893 ATOM 1117 С 3.758 1.00 24.85 VAL A 158 25.732 14.266 MOTA 1118 0 3.111 1.00 30.96 15.512 MOTA 1119 CB VAL A 158 27.954 5.217 1.00 27.87 28.751 14.595 CG1 VAL A 158 10 ATOM 1120 4.238 1.00 40.51 CG2 VAL A 158 27.791 16.704 MOTA 1121 4.399 1.00 34.39 1122 **GLY A 159** 27.483 12.956 MOTA N 3.016 1.00 CA **GLY A 159** 26.713 12.774 1.732 ATOM 1123 1.00 6.20 25.734 11.797 MOTA 1124 С **GLY A 159** 1.487 1.00 25.732 10.704 O **GLY A 159 15** ATOM 1125 0.848 1.00 ASP A 160 25.052 1126 N 11.441 MOTA 2.643 1.00 8.53 CA **ASP A 160** 24.106 10.302 MOTA 1127 2.828 1.00 11.97 ATOM 1128 C **ASP A 160** 22.755 10.698 2.177 1.00 14.44 1129 ATOM 0 **ASP A 160** 21.928 11.398 2.692 1.00 10.21 20 ATOM 1130 CB ASP A 160 24.037 9.829 4.277 1.00 12.43 MOTA 1131 CG **ASP A 160** 23.126 8.629 4.261 1.00 20.99 MOTA 1132 OD1 ASP A 160 22.525 8.408 3.179 1.00 33.03 MOTA 1133 OD2 ASP A 160 22.956 7.840 5.216 1.00 10.13 ALA A 161 22.455 10.402 ATOM 1134 N 0.961 1.00 12.33 **25** атом 1135 CA **ALA A 161** 21.318 10.743 0.269 1.00 11.01 MOTA 1136 C ALA A 161 19.961 10.317 0.848 1.00 15.22 MOTA 1137 0 ALA A 161 18.969 11.034 0.594 .1.00 9.50 ALA A 161 21.365 10.334 MOTA CB 1138 -1.172 1.00 13.68 VAL A 162 19.915 9.468 ATOM 1139 N 1.840 1.00 14.54 30 ATOM VAL A 162 9.014 1140 CA 18.653 2.287 1.00 9.86 1141 C **VAL A 162** 18.235 10.063 ATOM 3,258 1.00 13.50 o VAL A 162 17.094 10.458 MOTA 1142 3.377 1.00 20.47 18.596 7.778 MOTA 1143 CB **VAL A 162** 3.117 1.00 7.34 CG1 VAL A 162 18.931 6.592 1.00 6.50 **ATOM** 1144 2.259 35 ATOM 1145 CG2 VAL A 162 19.514 7.858 4.210 1.00 18.46 19.198 CYS A 163 10.733 ATOM 1146 N 3.719 1.00 13.44 **MOTA** 1147 CA CYS A 163 18.864 11.811 4.720 1.00 11.26 ATOM CYS A 163 18.256 12.963 1148 C 4.042 1.00 15.57 ATOM 1149 O CYS A 163 18.219 13.857 4.880 1.00 14.09 MOTA CB CYS A 163 20.144 12.145 1150 5.570 1.00 18,70 MOTA SG CYS A 163 20.748 10.705 1151 6.581 1.00 13.38 MOTA 1152 N THR A 164 18.100 13.014 2.696 1.00 21.82 MOTA 1153 CA THR A 164 17.603 14.283 2.171 1.00 23.08 16.597 **ATOM** 1154 С THR A 164 14.022 1.098 1.00 23.39 THR A 164 16.517 14.727 ATOM 1155 0 0.137 1.00 33.37 MOTA 1156 CB THR A 164 18.463 15.341 1.454 1.00 23.25 MOTA THR A 164 19.486 14.707 1157 OG1 0.674 1.00 23.21 **ATOM** 1158 CG2 THR A 164 18.958 16.261 2.491 1.00 37.71 ATOM **GLY A 165** 15.802 13.085 1159 N 1.309 1.00 24.23 MOTA **GLY A 165** 14.606 12.783 1160 CA 0.579 1.00 26.69 MOTA **GLY A 165** 14.699 11.814 1161 C -0.515 1.00 28.56 MOTA **GLY A 165** 13.680 11.775 1162 0 -1.124 1.00 39.76 MOTA 1163 N THR A 166 15.661 11.044 -0.736 1.00 25.80

ATOM 1164 CA THR A 166 16.006 10.220 -1.774 1.00 25.53 ATOM 1165 C THR A 166 16.195 8.866 -1.175 1.00 25.35 **ATOM** 1166 THR A 166 16.913 8.760 -0.206 1.00 30.91 MOTA 1167 CB THR A 166 17.406 10.657 -2.230 1.00 31.57 OG1 THR A 166 **5 ATOM** 1168 17.105 11.788 -2.982 1.00 24.13 CG2 THR A 166 MOTA 1169 18.061 9.559 -2.983 1.00 34.67 1170 N LEU A 167 15.734 7.833 -1.817 MOTA 1.00 19.63 MOTA 1171 CA LEU A 167 16.219 6.552 -1.465 1.00 16.11 MOTA 1172 C **LEU A 167** 17.395 6.044 -2.300 1.00 19.87 **LEU A 167 10** ATOM 1173 0 17.265 4.869 -2.612 1.00 21.38 CB LEU A 167 15.086 5.624 -1.555 ATOM 1174 1.00 23.45 **ATOM** 1175 CG LEU A 167 14.123 5.773 -0.401 1.00 33.91 -0.793 12.969 4.908 MOTA 1176 CD1 LEU A 167 1.00 42.10 0.903 CD2 LEU A 167 14.776 5.385 1.00 25.86 1177 MOTA -2.507 1.00 21.67 ILE A 168 18.534 6.726 **15** ATOM 1178 N ILE A 168 19.608 6.051 -3.170 1.00 23.38 ATOM 1179 CA 5.585 -2.189 1.00 20.47 ATOM 1180 С ILE A 168 20.675 ATOM 6.541 -1.581 1.00 18.08 1181 ILE A 168 21.139 0 6.835 CB ILE A 168 20.254 -4.297 1.00 23.50 MOTA 1182 CG1 ILE A 168 21.232 7.874 -3.800 1.00 13.71 **20 ATOM** 1183 ATOM 1184 CG2 ILE A 168 19.445 7.627 -5.276 1.00 18.16 -4.804 MOTA 1185 CD1 ILE A 168 20.908 8.938 1.00 26.95 -2.394 1.00 18.32 MOTA 1186 N ILE A 169 21.396 4.478 22.554 4.448 -1.536 1.00 13.25 MOTA 1187 CA ILE A 169 **25** ATOM ILE A 169 23.924 4.662 -1.967 1.00 11.95 1188 С MOTA 1189 0 ILE A 169 24.615 3.942 -2.539 1.00 20.35 -0.499 ATOM 1190 CB ILE A 169 22.503 3.351 1.00 21.07 -0.655 **ATOM** 1191 CG1 ILE A 169 23.398 2.181 1.00 11.06 CG2 ILE A 169 21.122 -0.533 1.00 7.02 MOTA 1192 2.801 30 ATOM -1.587 1.00 32.83 1193 CD1 ILE A 169 22.581 1.266 24.570 -1.296 1.00 17.16 MOTA 1194 N THR A 170 5.586 THR A 170 25.883 6.217 -1.397 1.00 13.01 ATOM 1195 CA ATOM 1196 THR A 170 26.722 5.719 -0.240 1.00 10.14 C 5.036 0.758 1.00 9.98 MOTA 1197 THR A 170 26.334 MOTA 1198 THR A 170 25.623 7.713 -1.344 1.00 15.02 CB ATOM 1199 OG1 THR A 170 26.466 7.947 -0.255 1.00 23.39 MOTA MOTA 1.00 41.10 1200 CG2 THR A 170 24.389 7.914 -0.452 MOTA -0.469 1201 N PRO A 171 28.000 5.738 1.00 10.12 MOT 5.066 0.339 1.00 11.88 29.012 1202 CA PRO A 171 MOTA PRO A 171 28.897 5.492 1.765 1.00 9.74 1203 С MOTA 1204 PRO A 171 28.904 4.682 2.646 1.00 9.54 0 5.207 MOT PRO A 171 -0.286 1.00 7.15 1205 CB 30.414 5.603 PRO A 171 30.017 -1.654 1.00 7.18 1206 CG PRO A 171 28.667 6.233 -1.601 1.00 6.90 1207 CD N ALA A 172 28.725 6.718 1.980 1.00 6.71 1208 1209 CA ALA A 172 28.247 7.315 3.169 1.00 8.62 С ALA A 172 27.075 6.631 3.892 1.00 10.99 1210 6.755 5.165 1.00 16.49 1211 0 ALA A 172 27.037 ALA A 172 27.904 8.812 3.040 1.00 2.86 1212 CB HIS A 173 26.287 5.815 3.278 1.00 6.36 1213 N 1214 CA HIS A 173 25.133 5.468 4.081 1.00 5.29 25.685 4.314 4.888 1.00 10.58 1215 C HIS A 173 25.082 3.598 5.668 1.00 9.36 1216 0 HIS A 173

D. SLK, 1998-12-04

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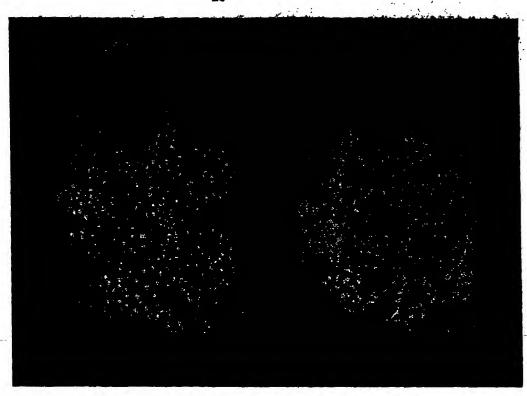
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	MOTA	1219	ND1	HIS A	173	22.066	5.327	4.565	1.00	8.48
	MOTA	1220	CD2	HIS A	173	22.148	3.264	3.670	1.00	7.83
5	ATOM	1221		HIS A		20.932	4.657	4.861	1.00	
•	ATOM	1222		HIS A		20.945	3.423	4.379	1.00	5.29
	ATOM	1223	N	LEU A		26.823	3.947	4.326	1.00	8.03
	MOTA	1224	CA	LEU A		27.344	2.623	4.682	1.00	B.06
	ATOM	1225	c.	LEU A		28.171	2.787	5.930	1.00	
10	ATOM	1226	0	LEU A		28.609	1.648	6.151	1.00	
10	ATOM	1227	СВ	LEU A		28.078	2.118	3.488	1.00	
	ATOM	1228	CG	LEU A		27.560	0.902	2.847	1.00	
				LEU A		26.024	1.017		1.00	
	MOTA	1229		LEU A				2.796		
45	ATOM	1230	_			27.913	0.740	1.421	1.00	
13	ATOM	1231	N	SER A		28.290	3.989	6.447	1.00	
	ATOM	1232	CA	SER A		29.230	4.052	7.553	1.00	
	ATOM	1233	C	SER A		28.872	4.811	8.847	1.00	
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20	MOTA	1236	OG	SER A		30.834	5.907	7.293	1.00	
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1	MOTA	1238	CA	TYR A		28.092	4.530	11.133		12.54
1	MOTA	1239	С	TYR A		28.530	3.671	12.272		11.16
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25	MOTA	1241	CB	TYR A		26.511	4.283	11.053	1.00	9.13
1	MOTA	1242	CG	TYR A	176	25.831	5.525	10.029	1.00	5.03
1	MOTA	1243	CD1	TYR A	176	25.874	6.923	10.425	1.00	2.75
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1	MOTA	1245	CE1	TYR A	176	25.287	7.754	9.633	1.00	4.25
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1	MOTA	1247	CZ	TYR A	176	24.658	7.329	8.399	1.00	6.22
	ATOM	1248	OH	TYR A	176	24.074	8.375	7.635	1.00	5.76
1	MOTA	1249	N	THR A	177	29.430	2.685	12.167	1.00	10.72
1.	MOTA	1250	CA	THR A	177	29.797	1.854	13.284	1.00	13.31
33	MOTA 6	1251	C	THR A	177	30.516	2.659	14.320	1.00	12.46
	MOTA	1252	0	THR A	177	30.311	2.436	15.475	1.00	13.12
	MOTA	1253	CB	THR A	177	30.658	0.683	12.798	1.00	3.49
1	MOTA	1254	OG1	THR I	177	31.361	1.247	11.870	1.00	32.08
3	ATOM	1255	CG2	THR A	177	29.675	-0.149	12.083	1.00	
7	MOTA 0	1256	N	ILE A	178	31.409	3.474	13.920	1.00	10.48
	ATOM	1257	CA	ILE A	178	32.203	4.246	14.783	1.00	15.25
4	ATOM	1258	C	ILE A	178	31.180	5.045	15.632	1.00	16.95
3	ATOM	1259	0	ILE A	178	31.092	4.774	16.851	1.00	22.68
	MOTA MOTA	1260	CB	ILE 2	A 178	33.338	5.121	14.357	1.00	25.11
3	MOTA	1261	CG1	ILE A	178	34.701	4.496	14.056	1.00	25.05
4	MOTA	1262	CG2	ILE A	A 178	33.599	6.205	15.392	1.00	27.60
	MOTA	1263	CD1	ILE A	A 178	34.553	3.006	14.071	1.00	55.86
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4	АТОМ	1265	CA	GLU A		29.290	6.610	15.985	1.00	16.94
1	MOT	1266	С		A 179	28.324	5.713	16.692	1.00	14.79
1	MOT	1267	0		A 179	27.683	6.012	17.716		19.20
	MOT	1268	СВ		A 179	28.555	7.637	15.169		21.16
2	MOT	1269	CG		A 179	28.790	7.283	13.691		50.37
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6000, SLK, 1998-12-04

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	MOTA	1379	CD1	ILE A	A 192	20.418	2.954	29.019	1.00.21 by
5	MOTA	1380	N	ARG A	A 193	20.535	7.574	32.629	1.00 28.72
	MOTA	1381	CA	ARG Z	A 193	20.800	B.068	33.963	1.00 33.95
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10	ATOM	1385	CG	ARG .	A 193	23.096	6.896	34.100	1.00 39.38
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15		1390	NH2	ARG	A 193	27.120	4.536	33.652	1.00 74.00
	MOTA	1391	OT	ARG	A 193	19.292	10.277	34.082	1.00 38.80
I	TER								
1									



pg. 2

Structure of cutinases from *F. solani pisi* (left) and *H. insolens* (right)

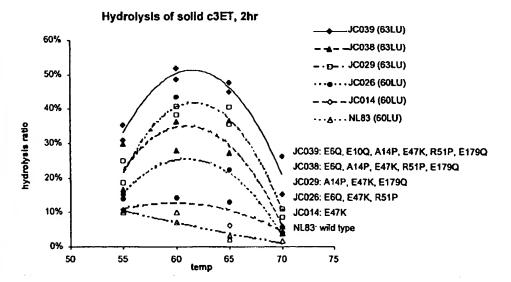


Fig. 3 Hydrolysis of solid c3ET, 2 hr

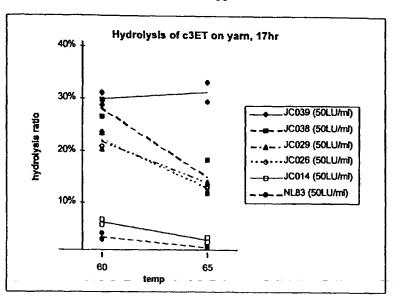


Fig. 4 Hydrolysis of c3ET on yarn, 17 hr

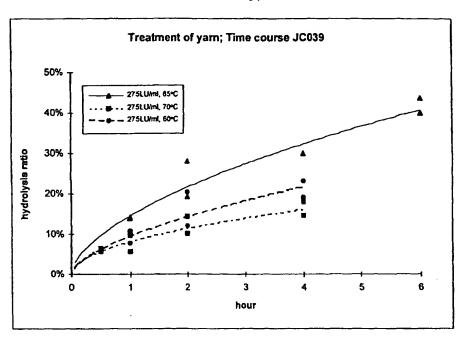
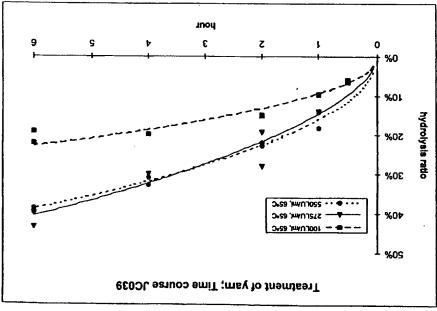


Fig. 5
Treatment of yarn; time course for JC039

9 .gi3





Treatment of yarn; time course for JC039

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